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PREFACE

This second edition has included six additional contributions and some contributions appeared in the first edition have been revised by the authors. An ISBN number has also been acquired for this volume.

Mathematical models are developed to approximate engineering, physical, environmental, social, and economic phenomena of various complexities. To ensure a correct use of a model, an appreciation of the relationship between (model) input factors and (model) output is of fundamental importance. The process aiming to understand how a model behaves in response to changes in its inputs is known as Sensitivity Analysis. Sensitivity Analysis applies to a variety of settings and fields. A large number of different methodologies, developed by scientists from a wide spectrum of disciplines, can be found in the literature.

In September 1995, the Joint Research Centre (Ispra) organised the first international symposium on Sensitivity Analysis of Model Output (SAMO95). SAMO95 was successful in bringing together researchers from different scientific backgrounds, involved in theoretical and practical aspects of sensitivity analysis, and offered a review of the current state of this art. The second international symposium, SAMO98, is organised by the Sensitivity Analysis group at the Institute for Systems Informatics and Safety, JRC and by the University of Venice.

Over 150 scientists from different disciplines and countries contribute to SAMO98 by presenting achievements, either in theoretical developments or practical applications. The final programme of the symposium includes nearly 50 oral presentations, organised into 13 thematic sessions, and 2 poster sessions, with over 30 contributions. An extended abstract of each presentation and poster is contained in the present volume. The number of participants and the variety of works presented at SAMO98 confirm the growing importance of Sensitivity Analysis in all settings and fields where modelling applies.

Readers of this volume might be interested in a special issue[1] based on SAMO98, where some selected topics addressed at the symposium are dealt with more in depth. The topics include SA applications to expert elicitation procedures within the Bayesian context, efficient input-output model representations, variance decomposition methods and their applications, hybrid approaches to SA, identification of model behaviour in the vicinity of extremes, generalised sensitivity analysis (related to Monte Carlo filtering), advanced model representations such DBM (Data Based Mechanistic) modelling, local automated SA (to compute large sensitivity matrices) and uncertainty in performance assessment.

[1] Saltelli, A., Chan, K., Scott, M. (Editors), Special Issue on Sensitivity Analysis, *Computational Physics Communication*, expected to appear in February 1999.

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A SENSITIVITY ANALYSIS OF A BAYESIAN APPROACH TO THE ESTIMATION OF SENSITIVITY AND SPECIFICITY OF DIAGNOSTIC TESTS IN THE ABSENCE OF A GOLD STANDARD

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1 INTRODUCTION

The absence of a Gold standard is often a limiting factor in evaluating the performance of a new diagnostic test. Comparisons of the new test may be made against existing methods and there may be a body of opinion available about the performance of those methods. Incorporating subjective opinion with observed performance to give an amalgamation of knowledge is, in broad terms at least, the essence of the Bayesian approach to Statistical Inference.

2 GIBBS SAMPLING FOR TWO TESTS

Joseph et al [1] proposed such an approach to evaluating the Sensitivity and Specificity of two diagnostic tests for *Strongyloides* infection The data were compiled from a survey of 162 Cambodian refugees who arrived in Montreal, Canada between July 1982 and February 1983. Two tests were involved, a serological test and a stool examination, and the numbers of patients classified as positive by either both tests, one or neither test formed the basic data. Opinion on the sensitivity, specificity and prevalence of the two methods was collected from a panel of experts from the McGill Center for Tropical Diseases. Beta distributions were then fitted to the experts numerical estimates of these parameters and these were then used as the prior distributions in the subsequent Bayesian analysis. Binomial distributions were then assumed for the numbers of true positives amongst the four categories of patients, those positive or negative on both tests and those negative on one test but not on the other. Because these crucial results were, by the very nature of the problem, unobservable, a Gibbs sampling approach was then used to form numerical estimates of the posterior distributions of sensitivity and specificity for each test together with prevalence and other derived statistics.

The two tests will be referred to as 1 and 2 with corresponding sensitivity, S_1 and S_2 , and specificity, C_1 and C_2; prevalence will be denoted by π.The observed number of patients in each of the four categories will be denoted by O_{++} , O_{+-} ,O_{-+} ,O_{--} with subscripts indicating the outcome of tests 1 and 2 respectively. The true positives will similarly be denoted by T_{++} ,T_{+-} ,T_{-+} ,T_{--} . Under the assumption of independence of outcome of the two tests, Table 1 gives the probabilities of the four possible outcomes of the two tests - note that the same probabilities can be achieved with sensitivities $1-C_1$,$1-C_2$, specificities $1-S_1$, $1-S_2$, and prevalence $1-\pi$.

Table 1: Probabilities of outcomes for two tests.

	Test 2 = +	Test 2 = -
Test 1 = +	$S_1S_2\pi + (1-C_1)(1-C_2)(1-\pi)$	$S_1(1-S_2)\pi + (1-C_1)C_2(1-\pi)$
Test 2 = -	$(1-S_1)S_2\pi + C_1(1-C_2)(1-\pi)$	$(1-S_1)(1-S_2)\pi + C_1C_2(1-\pi)$

Assuming Beta prior distributions for S_1,S_2,C_1,C_2 and π with parameters α and β suitably subscripted, the resulting posterior distributions are given in Table 2.

Table 2: Posterior distributions for two tests

	Posterior distribution
T_{++}	$\text{Bin}(O_{++}, S_1S_2\pi / (S_1S_2\pi + (1-C_1)(1-C_2)(1-\pi)))$
T_{+-}	$\text{Bin}(O_{+-}, S_1(1-S_2)\pi / (S_1(1-S_2)\pi + (1-C_1)C_2(1-\pi)))$
T_{-+}	$\text{Bin}(O_{-+}, (1-S_1)S_2\pi / ((1-S_1)S_2\pi + C_1(1-C_2)(1-\pi)))$
T_{--}	$\text{Bin}(O_{--}, (1-S_1)(1-S_2)\pi / ((1-S_1)(1-S_2)\pi + C_1C_2(1-\pi)))$
π	$\text{Beta}(T_{++}+\alpha_\pi, O_{--} - T_{++}+\beta_\pi)$
S_1	$\text{Beta}(T_{+-}+\alpha_{S1}, T_{--}+\beta_{S1})$
S_2	$\text{Beta}(T_{-+}+\alpha_{S2}, T_{--}+\beta_{S2})$
C_1	$\text{Beta}(O_{--} - T_{--}+\alpha_{C1}, O_{+-} - T_{+-}+\beta_{C1})$
C_2	$\text{Beta}(O_{--} - T_{--}+\alpha_{C2}, O_{-+} - T_{-+}+\beta_{C2})$

(The dot notation has been used to indicate totals of Ts or Os over both subscripts, e.g. $T_{+-}=T_{++}+T_{+-}$.)

The outcome of a Gibbs Sampling approach to this problem is most clearly illustrated by using the hypothetical set of data given below which represent expected values when $\pi = S_1 = S_2 = C_1 = C_2 = 0.9$ or $\pi = S_1 = S_2 = C_1 = C_2 = 0.1$.

Table 3: Hypothetical data

	Test 2 = +	Test 2 = -
Test 1 = +	73	9
Test 2 = -	9	9

Figure 1 illustrates the posterior distributions of prevalence and sensitivity and specificity of the two tests after starting with uniform priors on each of these unknowns; the BUGS 0.5 software of Spiegelhalter et al. [2] was used to carry out the computations.

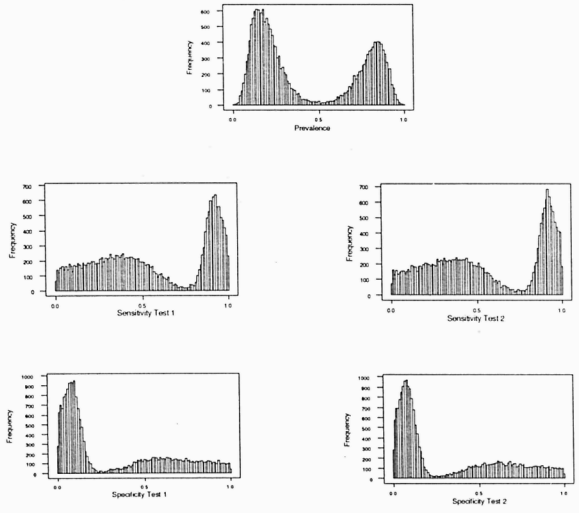

Figure 1: Posterior distributions with true values at 0.9 or 0.1.

The mean values of these posterior distributions are 0.43, 0.57, 0.57, 0.31, and 0.31 respectively, which conceal the actual nature of the distributions. Evidence of the imprecision is conveyed in the 95% credible intervals which are (0.07 - 0.92), (0.04 - 0.99), (0.03 - 0.99), (0.01 - 0.95) and (0.01 - 0.95). Clearly the existence of two feasible sets of sensitivity, specificity and prevalence for the same data together with a uniform prior has led to these bimodal posteriors, emphasising the need to look at the whole posterior distribution and not just summary statistics. That the two sets are extremely different allows the effect to be seen most clearly but in practice the two feasible sets are liable to be more similar. Figure 2 illustrates the outcome from a similarly generated set of data with sensitivity, specificity and prevalence set at 0.6 (or 0.4). Again with uniform priors the figure gives the posterior for the Sensitivity of Test 1; the posterior mean is 0.52 and the 95% credible interval is (0.03 - 0.94). There is clearly considerable scope for misinterpretation from such a posterior distribution.

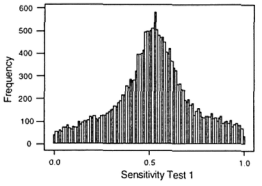

Figure 2: Posterior distribution with true values at 0.6 or 0.4

3 GIBBS SAMPLING FOR THREE TESTS

A similar problem arose in the evaluation of a whole blood near patient test (NPT) for *Helicobacter pylori*. However two reference methods were available for comparison with the NPT, the Helisal ELISA and the Helico G, and a literature search was used to establish the prior distributions of sensitivity and specificity for the three tests, and also for the prevalence. The observed data were the numbers of patients showing positive on both, one or neither of the NPT and each of the reference methods; 311 patients were involved. Extending the methodology of Joseph et al [1] to simultaneously analyse data from all three tests (eight data values as opposed to four) gives the posterior distributions given in Table 4, using an analogous notation.

Table 4: Posterior distributions for three tests

	Posterior distribution
T_{+++}	$\text{Bin}(O_{+++}, S_1S_2S_3\pi / (S_1S_2S_3\pi + (1-C_1)(1-C_2)(1-C_3)(1-\pi)))$
T_{++-}	$\text{Bin}(O_{++-}, S_1S_2(1-S_3)\pi / (S_1S_2(1-S_3)\pi + (1-C_1)(1-C_2)C_3(1-\pi)))$
T_{+-+}	$\text{Bin}(O_{+-+}, S_1(1-S_2)S_3\pi / (S_1(1-S_2)S_3\pi + (1-C_1)C_2(1-C_3)(1-\pi)))$
T_{+--}	$\text{Bin}(O_{+--}, S_1(1-S_2)(1-S_3)\pi / (S_1(1-S_2)(1-S_3)\pi + (1-C_1)C_2C_3(1-\pi)))$
T_{-++}	$\text{Bin}(O_{-++}, (1-S_1)S_2S_3\pi / ((1-S_1)S_2S_3\pi + C_1(1-C_2)(1-C_3)(1-\pi)))$
T_{-+-}	$\text{Bin}(O_{-+-}, (1-S_1)S_2(1-S_3)\pi / ((1-S_1)S_2(1-S_3)\pi + C_1(1-C_2)C_3(1-\pi)))$
T_{--+}	$\text{Bin}(O_{--+}, (1-S_1)(1-S_2)S_3\pi / ((1-S_1)(1-S_2)S_3\pi + C_1C_2(1-C_3)(1-\pi)))$
T_{---}	$\text{Bin}(O_{---}, (1-S_1)(1-S_2)(1-S_3)\pi / ((1-S_1)(1-S_2)(1-S_3)\pi + C_1C_2C_3(1-\pi)))$
π	$\text{Beta}(T_{\cdot\cdot\cdot} + \alpha_\pi, O_{\cdot\cdot\cdot} - T_{\cdot\cdot\cdot} + \beta_\pi)$
S_1	$\text{Beta}(T_{+\cdot\cdot} + \alpha_{S1}, T_{-\cdot\cdot} + \beta_{S1})$
S_2	$\text{Beta}(T_{\cdot+\cdot} + \alpha_{S2}, T_{\cdot-\cdot} + \beta_{S2})$
S_3	$\text{Beta}(T_{\cdot\cdot+} + \alpha_{S3}, T_{\cdot\cdot-} + \beta_{S3})$
C_1	$\text{Beta}(O_{\cdot\cdot\cdot} - T_{\cdot\cdot\cdot} + \alpha_{C1}, O_{+\cdot\cdot} - T_{+\cdot\cdot} + \beta_{C1})$
C_2	$\text{Beta}(O_{\cdot\cdot\cdot} - T_{\cdot\cdot\cdot} + \alpha_{C2}, O_{\cdot+\cdot} - T_{\cdot+\cdot} + \beta_{C2})$
C_3	$\text{Beta}(O_{\cdot\cdot\cdot} - T_{\cdot\cdot\cdot} + \alpha_{C1}, O_{\cdot\cdot+} - T_{\cdot\cdot+} + \beta_{C1})$

With seven variables underlying the eight data values the problems noted earlier, when four data values were associated with five variables, might be expected to have been avoided. There also exists the possibility of examining the three comparisons of pairs of tests. The observed data for Helicobacter are presented in Table 5.

Table 5: Helicobacter results using three tests.

	Helisal = +		Helisal = -	
	Helico G = +	Helico G = -	Helico G = +	Helico G = -
NPT = +	173	9	5	13
NPT = -	21	6	25	59

Resulting 95% credible intervals from the separate analyses of data from pairs of tests and all three tests are given in Table 6.

Table 6: Posterior 95% credible intervals using the data in Table 5.

	NPTvHG	NPTvHS	HGvHS	NPTvHGvHS
NPT	0.80 - 0.97	0.86 - 0.98		0.84 - 0.94
Sensitivity HG	0.87 - 0.96		0.90 - 0.97	0.90 - 0.96
HS		0.89 - 0.97	0.88 - 0.97	0.93 - 0.98
NPT	0.76 - 0.98	0.81 - 0.99		0.77 - 0.91
Specificity HG	0.58 - 0.90		0.68 - 0.92	0.64 - 0.81
HS		0.74 - 0.95	0.81 - 0.97	0.82 - 0.96
Prevalence	0.54 - 0.76	0.58 - 0.72	0.61 - 0.74	0.59 - 0.70

Examination of the sensitivity of this methodology is ongoing but it would appear that this particular approach to the problem of testing in the absence of a gold standard is improved by comparison of the method under test to two reference methods rather than one.

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SAMPLE2: SOFTWARE TO GENERATE EXPERIMENTAL DESIGNS FOR LARGE SENSITIVITY ANALYSIS EXPERIMENTS

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1 INTRODUCTION

The secret of efficient sensitivity analysis lies in the choice of experimental design. In modelling situations where the number of parameters is large (e.g., more than 100), a very large number of randomly-chosen model evaluations may be required to explore the influence of each parameter. Fewer evaluations are needed if the goal is restricted to identifying and investigating only the most influential parameters. In fact, proper design of the experiments to be performed can reduce the number of experiments required to a number that is smaller than the number of parameters ("supersaturated" designs). Experimental designs can be used only in situations where the model can be evaluated for any selected combination of parameter values; this is frequently the case with computer models. Experimental designs are effective in sensitivity analysis because they can increase the amount of useful information in a simulation dataset, under reasonable assumptions.

Andres [1] showed how to generate experimental designs with a variety of useful features that up to that time had not been investigated. The research code SAMPLE was developed in 1989 (and later enhanced in 1991) to implement the techniques of the earlier paper. SAMPLE itself has never been described in print, but papers describing its use [2-4] showed the effectiveness of sensitivity analysis with iterated fractional factorial designs (IFFDs) generated by SAMPLE, particularly in screening hundreds or thousands of parameters. A SAMO'95 paper described the algorithms behind SAMPLE in the form of Mathematica scripts [5].

SAMPLE2 is a new version of SAMPLE that incorporates several improvements over the original. Its features are described in this paper.

2 SAMPLES

SAMPLE2 generates samples from a sample space consisting of all possible combinations of parameter values that can occur in a model. A sample can be thought of as a large rectangular matrix **B** with R rows and C columns. Each column represents a parameter. Each row represents an experiment. The value in the (i,j)'th position of **B**, B_{ij}, is the value to be assigned in the i'th experiment to the j'th parameter of a model. By convention, all parameters lie in the closed interval [0,1]. If parameters are needed in a different range for a particular model, parameter values are transformed to the appropriate domains after the sample is generated.

A sample description consists of two parts, the experimental design, and the parameter rule set. The experimental design determines a matrix **A**, with the same shape as **B**. **B** is obtained from **A** by performing parameter-specific transformations according to the parameter rule set.

3 EXPERIMENTAL DESIGNS

SAMPLE2 supports several types of experimental designs to generate a design matrix **A**. The following options are available for the columns of **A**:

1. Pseudorandom designs. First a simple random design is generated for the column such that each value is independently and uniformly distributed on the half-open interval [0,1). This initial value can be subsequently modified, depending on several settings:

    - Number of levels. A simple random design can be thought of as a latin hypercube design (i.e., a stratified design in which every parameter is stratified independently) with only one level or stratum. All values are selected from the entire half-open interval [0,1). If the number of levels is a larger number L, then the values in the column are transformed by allocating an equal number of values to each equal-width level. For example, if L=2, then half the values come from [0,0.5) and half from [0.5,1). If L=R, then every value is selected from a different level. L must divide into R.

- Orthogonality. simple random and latin hypercube designs can exhibit spurious correlations among the parameters. An orthogonal 2-level fractional factorial design avoids spurious correlations by basing the pattern of high and low values for each parameter on a column of a standard Hadamard matrix. SAMPLE2 requires that R be a power of 2. An orthogonal 2-level fractional factorial design is also a latin hypercube design where L must be even, and at least 2.

- Folding. By default, each row of the matrix A is unique. In a folded design, each row is doubled, and the second copy of the row takes complementary values to the first. For example, if the value of parameter j in a particular row is 0.2239773, then the complementary value in the associated folded row is 1-0.2239773=0.7760227. Folding can translate a "Resolution III" fractional factorial design into a "Resolution IV" design [6].

2. Low-Discrepancy Sequences. Wozniakowski [7] proved that low-discrepancy sequences achieved the minimal average case complexity for multivariate integration of continuous functions. Sobol' [8] demonstrated the use of low-discrepancy sequences for sensitivity analysis. Sobol's sequences are rather complicated to generate [9], but Struckmeier [10] devised an algorithm for generating generalized Halton sequences as efficiently as pseudorandom numbers. For each parameter, randomness enters in the choice of starting value, in the choice of prime number, and in the number of points dropped from the start of the sequence.

4 RECURSIVE SUBDIVISION OF EXPERIMENTAL DESIGNS

Much of the advantage ascribed to IFFDs comes from a partitioning of the experimental design into subdesigns. The original SAMPLE supported simple random sampling at the global level, and one stage of subdivision. For the IFFD technique, each subdesign was either an orthogonal fractional factorial design, or a fractional factorial/latin hypercube design with stratification on more than 2 levels. SAMPLE2 supports recursive subdivision of some kinds of design, so that there can be more than 2 stages. In a partitioning, the number of rows in the entire design is broken up: $R=(R_1+R_2+...+R_S)$, where S is the number of subdesigns.

(1) Simple random design. A simple random design can be partitioned into parts with any of the kinds of designs described above. For example, a simple random design with R=80 experiments can be partitioned into 5 subdesigns, each of which is a fractional factorial design with 16 experiments. The original sampled values in the simple random design are used in calculating the new values in the subdesigns. SAMPLE2 requires that each subdesign be of the same type (i.e., simple random, latin hypercube or fractional factorial design or low-discrepancy sequence), but they can be of different sizes. The constraints mentioned above must be observed. For example, if the subdesigns are orthogonal, each of R_1, R_2, etc. must be a power of 2.

(2) Latin hypercube design. A latin hypercube design can be partitioned into subdesigns that are latin hypercube or fractional factorial/latin hypercube designs. The number of rows R_k of each subdivided design must divide evenly into R. Each subdivided design must have a number of levels L_k that divides into R_k, and is at least as large as the lesser of L and R_k, for k from 1 to S. If the original design had $L=R$ (i.e., exactly one value in each level of the design), and each subdesign has $L_k=R_k=R/S$, then this single design achieves two objectives: (a) achieving the full advantage of using a large latin hypercube design, which could approach the asymptotic behaviour described by Stein [11], and (b) replicating the smaller latin hypercube design to get estimates of sample variability. This approach is most effective when the subdesigns are also orthogonalized to fractional factorial/latin hypercube designs.

(3) Folded design. Each subdesign of a folded design must also be folded, and hence must have an even number of rows.

(4) Fractional factorial design, low-discrepancy sequence. At this time, fractional factorial designs and low-discrepancy sequences cannot be subdivided by SAMPLE2.

5 PARAMETER RULE SET

Rules can be provided for each parameter to transform the values in the matrix **A** into modified values in the matrix **B**. Two types of transformation are supported in SAMPLE2:

(1) Importance. To emphasize sampling from one of the ends of the interval [0,1], values can be transformed towards one end or the other. This transformation affects the weighting to be used for each experiment in integration and sensitivity analysis.

(2) Discretization. (Discretization follows importance transformation.) For example, in an orthogonal design, each value in [0,0.5) can be transformed to 0 and each value in [0.5,1) can be transformed to 1. This method can be used to generate a standard fractional factorial design. In general, a unique value can be assigned to each level of a latin hypercube design. Other types of discretization are occasionally useful.

6 128-BIT PSEUDORANDOM GENERATOR

Since random sampling and randomized transformations are so important for the operations of SAMPLE2, a 128-bit pseudorandom number generator [12] has been adapted for use in SAMPLE2. It is designed to support up to 2 billion different samples, each of which can have up to 2 billion independent parameters, each parameter having hundreds of millions of values. Statistical properties have been checked theoretically and empirically and found to be excellent [12].

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EVALUATING UNCERTAINTIES IN TURBULENT CONVECTION MODEL USING TWO DIFFERENTIAL ANALYSIS METHODS.

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We cannot be content in general with results from models more and more complex and detailed. We wish also evaluate the reliability domain that are associated with the results of simulations due to uncertainties and numerical approximations.

In this paper, authors propose an extended protocol to calculate uncertainties for long-running time simulations such as the computational fluid dynamics program BRIVE-CFD (1). Main idea is that computational and experimental results should have an uncertainties domain attached to the reference values. The reliability domain of experimental measurements are systematic. It is uncommon to found numerical results with uncertainties. The authors compare two determinist methods to calculate uncertainty domain for numerical simulations.

First part of the study presents an application involving an air convection model in large enclosure such as the rooms of buildings (figure 1). This enclosure is rectangular, and the air flow in the cell is turbulent. The fluid is injected into the cavity with two profiles (plane and parabolic). A draining hatch is located on the opposite face. The geometrical caracteristics are known with a hight accuracy. The computational program uses a k-epsilon model to solve the turbulent flow in the bidimensional cavity. The observed output are the field of respectively the horizontal and vertical speed, the speed modulus, the turbulent kinetic energy k, the turbulent kinetic energy dissipation rate ε and the turbulent viscosity. Using this program, we calculate, in a first simulation, physical parameters of the air flow, named central values or references values.

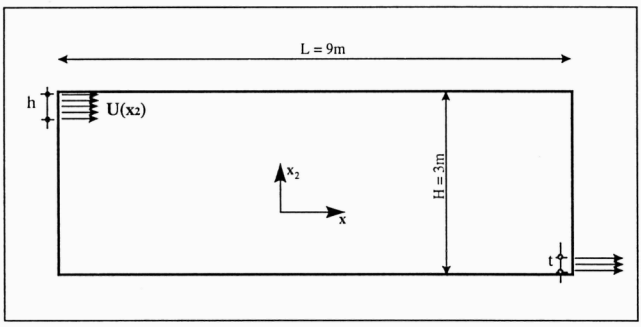

Figure 1: The two-dimensional ventilated enclosure studied.

In the second part, we compute the uncertainties domain for each parameter. The data assumed to be known with uncertainty are the injection speed, the turbulent injection strenght and the air cinematic viscosity. Two differential methods are then used and avoid intensive computation with a Monte-Carlo method. We show how we validate a differential method which allows large savings in computation time. The Finite Differences Differential Analysis method FDDA (2) and Quasi-Analytical Differential Analysis method QADA (3) give us the reliability domain of the output S_k

according to the uncertainties of the inputs e_j and control parameters c_i with respectively k = 1, ... , n , j = 1, ... , p and i = 1, ... , m. In our notation, inputs are time dependant and parameters are time independant.

The relation between the uncertainties of output S_k and both inputs and control parameters is

$$\Delta S_k = \sum_{j=1}^{m} \left| \frac{\partial F_k}{\partial e_j} \right| \Delta e_j + \sum_{j=1}^{n} \left| \frac{\partial F_k}{\partial c_j} \right| \Delta c_j \qquad (1)$$

For our problem, we consider only the uncertainties of control parameters. They are time independent.
At the end, phenomena studied is not only represented by a simple value of curve, but by an uncertainty domain around his central value. A researcher then can report experimental values, with his experimental uncertainties, and compare the two domains relative position.

The two methods, on the other hand, involve different approaches. The first, a deterministic type (Finite Differences Differential Analysis, FDDA) gives us an numerical estimation of the partial derivatives. The second is also a deterministic type, but compute directly sensitivity coefficients. The parallel use of these methods has afforded us increased knowledge of benefit to users of calculation domain. The FDDA method has to be particularly dependable and effective. As regards dependability, we have observed in a previous study that the uncertainty interval described by this method almost systematically includes the values computed by the Monte-Carlo method. The model study was an convective - radiative thermal exchange program and was highly non-linear. In addition, this framing of the Monte-Carlo results by first order approximation of FDDA does not lead to an excessive extension of the area of uncertainty of the results, but on the contrary, narrows the extrema of the MC uncertain domain. The interval which the FDDA method leads to is therefore always more pessimistic than that obtained by the MC method, but the difference does not exceed 2% (figure 2). The application of FDDA first order approximation to the air convection model in large enclosure therefore proves to be satisfactory.

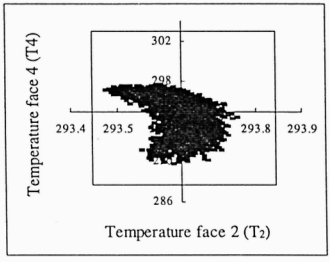

Figure 2 : Comparison between FDDA and MC methods on a highly non-linear convective - radiative thermal exchange model. This figure shows the uncertainties of two temperatures. The solid line gives the uncertainty domain computed with FFDA and the cloud of points gives the results of MC analysis.

As regards effectiveness, the calculation times necessary to obtain the uncertainty interval are far below those of the MC method (rate 1 to 100 in favour of FDDA). The computation of bidimensional turbulent air flow needs many iterations. The differential method obtain the reliability interval with the less numerical effort, whatever the slimness of mesh.

The only precaution necessitated by the FDDA method is within the determination of the calculation step of partial derivatives. For the nonlinear models (case of the turbulent air flow), the determination of the step requires close attention during the implementation of resolution algorithm procedures. The calculation step of partial derivatives must be dynamic, and different for each uncertain input parameter. We have developped an numerical algorithm which generates automatically the calculation step for a good estimation of partial derivatives. This is a characteristic of the FDDA method. But it is likely that in deterministic type approaches, a sequential analysis of the numerical and mathematical treatment of the model is essential. Nonetheless, when this is done, and the partial derivatives are coded, the uncertainty of the output vector is easily calculated. The computation cost depends on the number of parameters.

For m parameters, the FDDA method needs n + 1 simulations to compute partial derivatives of S_k with a non centered sheme.

The principal interest with the Quasi-Analytical Differential Analysis (QADA) is the direct calculation of sensitivity coefficients with only one simulation rather than the more expensive time cost require by FDDA. We have verified that major time savings can be obtained in the uncertainty analysis, especially when using a long-running time simulation as BRIVE-CFD (in 2 or 3D). However, the QADA is numerically more complex than the FDDA and needs the solution of a large system of linear equations. An adapted banded out of core solver is necessary (3).

Another considerable advantage of these two methods is the possibility of estimating explicitly the sensitivity of each output element on all of the input data. In our case, we show that the the injection speed and the turbulent injection strenght are the most influential parameters. Therefore it is possible to envisage using it inversely by transmitting information back to reduce the uncertainty of results or optimize the value of certain data. This strategic use of the methods can also be applied to the understanding of the consequences of a deviation of certain control parameters.

In the core region of the studied enclosure, the uncertainties concerning the turbulent kinetic energy, its dissipation rate and the turbulent viscosity are small. However, they are very large in the top left corner of the enclosure, in the vicinity of the inlet:

- turbulent kinetic energy: 40% or ± 20% for the plane profile at the inlet,
  120% or ± 60% for the parabolic profile at the inlet.

- dissipation rate of the turbulent kinetic energy : 50% or ± 25% for the plane profile at the inlet ,
  90% or ± 45% for the parabolic profile at the inlet.

In case of parabolic inlet velocity profile, these uncertainties are also large in the stagnant regions (top right and bottom left corners of the cavity).

For the two-dimensional ventilated enclosure, the uncertainties turn out to be large in the stagnant regions in the top right and bottom left corners, and in the jet region. To obtain accurate information on these regions, the prediction of the dynamic variables in the jet region needs to be improved, and perhaps also that of these variables in the stagnant regions.

Finally, we emphasize that these two methods impose *a priori* few restrictions concerning the nature and the amplitude of the uncertainties associated with data. The differential methods keep account caracteristics of numericals solvers in computational fluid dynamics field. This protocol remains compatible with all types of numerical programs. A choice must only be make within the FFDA, easy to implement but time-intensive computation and QADA, complex but time-saving because she needs only one simulation.

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STRUCTURAL ERROR AND THE IDENTIFICATION OF STRUCTURAL CHANGE{PRIVATE } IN THE BEHAVIOUR OF ENVIRONMENTAL SYSTEMS

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1 INTRODUCTION

Many models of the behaviour of environmental systems can be defined according to the following (lumped-parameter) representation of the state variable dynamics,

$$dx(t)/dt = f\{x,u,\alpha,t\} + \xi(t) \tag{1a}$$

with observed outputs being defined as follows,

$$y(t) = h\{x,\alpha,t\} + \eta(t) \tag{1b}$$

in which f and h are vectors of nonlinear functions, u, x, and y are the input, state, and output vectors, respectively, α is a vector of model parameters, ξ and η are notional representations respectively of those attributes of behaviour and output observation that are not to be included in the model in specific form, and t is continuous time. Of central concern in this paper is the challenge of coping with model identification and prediction when the content of $[x,\alpha,f,h]$ may appear to change with time (an essential element of ideas expressed on this matter at length elsewhere, [1]).

2 STRUCTURAL ERROR

In very broad terms, the choices of $[x,\alpha,f,h]$ signify that which we presume (or wish) to know of the system's behaviour, relative to the purpose of the model, while $[\xi,\eta]$ acknowledge in some form that which falls outside the scope, or below the resolving power, of the model. Much, of course, must be subsumed under the definitions of ξ and η. We may have chosen to exclude from the model some of that which was known beforehand (but which was judged not to be significant); there may be features for which there are no clear hypotheses (and therefore no clear mathematical expressions), other than that these may in part be stochastic processes with presumably quantifiable statistical characteristics; there may be yet other features of conceivable relevance, but of which we are simply ignorant; and, as is most familiar, there may be factors affecting the processes of observation such that we are unable to have uncorrupted, perfect access to knowledge of the values of the inputs, states, or outputs.

Thus, typically, *structural error* may be thought of as a measure of the extent to which the expression of what is "known", i.e., $[x,\alpha,f,h]$, diverges from the "truth". The term conceptual error has been used on occasion to represent much the same idea [2]. More generally, and more loosely, such things might be talked of as scientific uncertainties, which conventionally are reduced over successive generations of research programmes, as in the International Geosphere-Biosphere Programme (IGBP) of the International Council of Scientific Unions (ICSU). In other words, the intent – caricatured somewhat – is to expand the scope and refinement of $[x,\alpha,f,h]$ until the structural uncertainty of $[\xi,\eta]$ has been ground into insignificance. At any instant in this lengthy quest the current content of what is known can be used for the purposes of making predictions, which, astutely, may now be cloaked in the cautions of confidence bounds deriving from the various sources of uncertainty, including from $[\xi,\eta]$.

There are a number of bothersome points in this argument, however. First, the quest has no end; second, we are unable to quantify structural error, since the distance of the model's structure from the truth cannot, strictly speaking, be known; and third, of primary importance herein, we may be led to expect structural error to be revealed only in $[\xi,\eta]$. At some level of resolution, cutting out the representation of the system of interest and abstracting it away from its context in the seamless web of interactions in which it sits, requires a line to be drawn between that which we know and that of which we know little or nothing. In this, however, the phrase "at some level of resolution" is not as

innocuous as it may seem. For the resolving power of our models must always be bound to be macroscopic relative to reality. Except in the absolutely limiting case of a representation of behaviour purporting to describe the relationships among the elementary particles of the universe, the web of interactions of which we conceive cannot represent reality resolved at it finest degree. We have always thought of the parameters (α) of our models as *constants*, being invariant with time (and space); and to have arrived at relationships whose parameters can be identified from observed behaviour as indeed invariant is strongly suggestive of the fact that no more elementary description of that behaviour is tenable (or necessary). Yet in the relatively macroscopic representations we construct of the behaviour of environmental systems these parameters can be seen as merely coarse approximations of what we may suspect to be (in truth) more refined representations. Parameters at one (lower) level of resolution i, say α^i, may subsume under their definition a set of state variables and parameters $[x^{i+1},\alpha^{i-1}]$ at the next (higher) level of resolution, and so on, as the resolving power of the model is progressively increased [1,3]. We talk of *parameterising* those fine-grid features of behaviour that are too detailed to include in our current models. We should expect the structural error of so doing, in the light of the expectation that the values of x^{i+1} will not be invariant with time, to be revealed, in principle, as a nonstationarity in the reconstructed "behaviour" of α^i when attempts are made to reconcile the structure of the model with that underlying observed behaviour [4].

Structural error can therefore be revealed, again in principle, not only through the devices of $[\xi,\eta]$ but also through refutation of the assumption of invariance in the model's parameters $[\alpha]$. To achieve this requires us, first, to set aside the conventional prior assumption of α as a random variable and instead assume it to be a stochastic process and, second, to have available the algorithmic means to reconstruct its potential variations with time. Typically, filtering theory has been used to illuminate structural error in this manner [4]. One can make assumptions, *inter alia*, about the statistical properties of $[\xi,\eta]$ and then reconstruct both an innovations sequence, $\_(t_k \mid t_{k-1})$, i.e., a measure of the distance of the one-step-ahead predictions of the model from observed behaviour, together with the temporal sequence of the parameter estimates $(t_k \mid t_k)$, assuming the availability of observations at discrete sampling instants t_k.

This will not allow us to quantify the structural error in the model, for example, for the purposes of computing the propagation of prediction errors (as attempted in [5]). But that is not the question we are seeking to address herein. Rather, it is this: how can we discover the presence of a substantial and essentially non-random error in the structure of the model -- where it touches on the boundaries of what "we know we do not know" (our ignorance) -- especially in detecting a potential *change* of structure and in forecasting in the face of such structural change [1]?

3 STRUCTURAL CHANGE

The word "change" is clearly the key word here. To appreciate its significance it is worth quoting at length the following observations from Allen [6]:

> [I]f the world is viewed as some kind of 'machine' made up of component parts which influence each other through causal connections, then instead of simply asking how it 'works', evolutionary theory is concerned with how it got to be as it is.
>
> The Newtonian paradigm was not about this. It was about mechanical systems either just running, or just running down.
>
> The key issue is centred on the passage between detailed microscopic complexity of the real world, which clearly can evolve, and any aggregate macroscopic 'model' of this.
>
> The central question which arises is that in order even to think about reality, to invent words and concepts with which to discuss it, we are forced to reduce its complexity. We cannot think of the trillions of molecules, living cells, organisms, individuals and events that surround us, each in its own place and with its own history. We must first make a taxonomic classification, and we must also make a spatial aggregation.
>
> [I]f, in addition to our basic taxonomic and spatial aggregations, we assume that only average elements make up each category, and that only the most probable events actually occur, then our model reduces to a 'machine' which represents the system in terms of a set of differential equations governing its variables.
>
> But such a 'machine' is only capable of 'functioning', not of evolving. It cannot restructure itself or insert new cogs and wheels, while reality can!

What Allen imagines is the possibility of the structure of the web of interactions, of which we conceive in our models, dissolving, as it were, and then re-crystallizing into some other structure, with a different number of states and parameters and different inter-connections between the states. And what Allen asks is: can we discover the rules by which the system will re-structure itself?

We do not presume to answer such a question. Instead, we ask the questions: assuming the arrangement of the interactions among the state variables in the model is fixed and invariant, i.e., the content of $[f,h]$ is invariant, can we detect a change in those inter-connections, i.e., a change in α, and from this could we fathom a different implied number and arrangement of the system's state variables and their interactions? We argue that this is likely to be a real and common problem, because our models are bound to be approximations of the unknowable truth. What may appear to have dominated behaviour in the past -- from interpretation of the empirical record -- may decline into insignificance in the future. Conversely, what may previously have been below the resolving power of the model, buried perhaps in the residual noise of the historical observations, may come to dominate behaviour in the future. We might call this *apparent* structural change, brought about because the resolving power of our models can never be as fine-grained as that of the truth. We shall draw back therefore from addressing the problem of attempting to predict, in effect, the discrete event of the birth of a new state equation in the model, which is implied in Allen's question.

4 APPROACHES TO THE DETECTION OF STRUCTURAL CHANGE

For the purposes of the present paper our challenge has three parts to it. First, can we detect such a change of structure within the historical record of past behaviour? Second, could we parameterise this parametric change, for possible extrapolation into the future? And third, how might we organise our models in order to maximise the possibility of identifying potentially critical changes of structure in the future? Three lines of approach to answering these questions can be discerned, each with a slightly different conceptual basis in (a) filtering theory and recursive estimation, (b) control theory, and (c) a regionalised sensitivity analysis (RSA).

Filtering theory and recursive estimation. In a recursive, predictive world our previous model of the system's behaviour could be replaced by the following innovations form

$$d\boldsymbol{x}(t\,|\,t_{k-1})/dt = \boldsymbol{f}\{\boldsymbol{x}(t\,|\,t_{k-1}),\boldsymbol{u}(t),\alpha\} + \boldsymbol{K}\_(t\,|\,t_{k-1}) \qquad \textbf{(2a)}$$

$$\boldsymbol{y}(t_k) = \boldsymbol{h}\{\boldsymbol{x}(t_k\,|\,t_{k-1}),\alpha\} + \_(t\,|\,t_{k-1}) \qquad \textbf{(2b)}$$

in which the elements of the matrix $\boldsymbol{K}$ can be estimated as additional parameters, in the same spirit as previously for just the elements of α [7,8]. The divide between what we know (relatively well) and what we do not know (at all well) lies now, in part, between the first and second terms on the RHS of equation (2a). Thus, for example, if the reconstructed estimates of the elements of $\boldsymbol{K}$ were to veer away from essentially the value of zero -- as the historical record is processed sequentially -- this could imply that the one-step-ahead predictions of the model rest more on the unknown aspects of divergence between the immediate past predictions and observed behaviour, i.e., _, than on the supposedly known content of the model, symbolised by $[f,h]$. In other words, $\boldsymbol{K}$ allows us now to illuminate sources of structural change and error residing in the largely unknown, whereas nonstationary behaviour in the recursive estimates of α permits tracing of potential change within what was previously presumed known, i.e., prior theory. Further, since there is empirical evidence suggesting that *slow*, low-frequency change can be identified with α such as a changing land cover in a rainfall-runoff model of a hydrological catchment [9], it is possible that the identified variations in ^{i} could themselves be modelled, by invoking invariant parameters at a finer level of representation, i.e., α^{i+1}. This approximative model of the slowly evolving change of structure could then be extrapolated for uses underpinning the prediction of future behaviour [1].

Control theory. If there were no dividing line of the present (t) between the past (t^-) and the future (t^+), and if there were some specification of a target, desired (or feared) future to be reached (or avoided), say $x(t^+)$, we might be able to bend the conventional course of control theory towards a different purpose. For instead of asking, in equation (1a) or (2a), what choice of inputs $\boldsymbol{u}$ will transfer the state of the system from its observed past to this target future, subject to convenient assumptions about α (as in the formulation of policy for stabilising atmospheric CO_2 concentrations by the year 2300, say), we might enquire of what changes of α, subject to convenient assumptions about $\boldsymbol{u}$, would effect the same transfer. More specifically, the manner in which α must change in the vicinity of the present (t) in order to attain $x(t^+)$ in the future, given the state trajectory of the past, may provide clues as to where to look for incipient changes of structure.

Regionalised sensitivity analysis (RSA). All of the foregoing may appear attractive in principle. In practice, these approaches may either be restricted -- perhaps unsatisfactorily -- to success only in the case of very low-order models, or be rendered impotent by the substantial uncertainty so often attaching to the analysis of environmental systems. The real issue is, can one discover something of significance about what has governed, or what may come to govern, the

behaviour of the system in the midst of all the uncertainty? The RSA of Hornberger, Spear, and Young [10,11,12] calls for the model, i.e., $[x,\alpha,f,h]$, to be assembled as a rich composite of all the scientific partial knowns and unknowns constituting our current, best, quantitative representation of the system's behaviour. Uncertainty is recognised in both the bounds attaching to the possible ranges of values that may be assumed by α in the context of a Monte Carlo simulation and those categorising what was deemed to have been the behaviour of the past and what is desired/feared to become the behaviour of the future. There is no measure of the distance of the model from the truth in an RSA, only a 0/1 classification of a candidate parameterisation according to whether behaviour is given or not. The intent is to cast the net of the model sufficiently widely, yet finely, over the set of potentially important governing mechanisms; to identify the (hopefully) small sub-set of parameters, say α^K, that are absolutely critical to the task of discriminating between whether behaviour is given or not; and then to examine how the sub-sets of these key parameters differ between those critical to the matching of past behaviour, $\alpha^K(t^-)$, and those critical to attaining the target behaviour of the future, $\alpha^K(t^+)$. In other words, there is the possibility of identifying on which key scientific knowns/unknowns the reachability of the target future hinges. Structural change, as such, is not revealed through nonstationarity in estimates of the model's parameters, because some finer-scale representation has been overlooked, but through a change of "status" in an individual parameter, for example, through α_i, which was (was not) significant but may become insignificant (significant) in the future. We have thus far had some practical success with this form of computational analysis, in the closely related problem-setting of model validation and quality assurance [13].

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SENSITIVITY INDICES FOR (TREE-)DEPENDENT VARIABLES

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1 INTRODUCTION

In this paper we consider the sensitivity of a model f with respect to its parameters $x_1, \ldots x_n$. The model output will be considered as a function $f(x_1, \ldots, x_n)$. The values taken by the input variables are uncertain, and hence the values of f are uncertain too. Sobol [1] introduced sensitivity indices for the case in which the variables $x_1, \ldots, x_n$ are stochastically independent. In this paper we address the problem of sensitivity indices for dependent variables. We show that there are two distinct roles played by the sensitivity indices when the input variables are independent, but that when the input variables are dependent then two seperate types of index can be defined.

The new sensitivity indices that will be defined here can be calculated by Monte Carlo simulation in a similar fashion to the Sobol indices. In general it is difficult to estimate these indices efficiently as higher order indices require sampling from higher dimensional distributions. However, we show that if the dependence between the variables $x_1, \ldots x_n$ is described by a tree-dependent probability distribution (as used for example for dependence modelling in *Unicorn*, [2], an uncertainty analysis code developed at the TU Delft), then the Monte Carlo simulations required for calculating the indices can be done relatively efficiently. The higher-dimensional distributions required have themselves a tree structure that can be derived straightforwardly from the orginal tree structure of $x_1, \ldots x_n$.

2 SOBOL SENSITIVITY INDICES

The Sobol indices are based on a decomposition of the function f into functions of different dimensions: The representation

$$f(x_1, \ldots, x_n) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \ldots f_{1\ldots n}(x_1, \ldots, x_n)$$

is called a decomposition of summands of different dimensions if $\int f_{i_1\ldots i_k}(x_{i_1} \ldots x_{i_k})\, dx_{i_j} = 0$, for all $i_1 \ldots i_k$, for all j. The following properties hold for the decomposition: (i) The constant f_0 equals $\int f(\underline{x})\, d\underline{x}$; (ii) The functions $f_{i_1\ldots i_k}$ are orthogonal, that is $\int f_{i_1\ldots i_k}(x_{i_1} \ldots x_{i_k}) f_{j_1\ldots j_\ell}(x_{j_1} \ldots x_{j_\ell})\, d\underline{x} = 0$, whenever $i_1 \ldots i_k \neq j_1 \ldots x_{j_\ell}$; (iii) The decomposition in summands of different dimensions is unique.

We now define variances $D = \int f^2(\underline{x})\, d\underline{x} - f_0^2$, and $D_{i_1\ldots i_k} = \int f^2_{i_1\ldots i_k}\, dx_{i_1} \ldots dx_{i_k}$ for each $i_1 \ldots i_k$. The *Sobol sensitivity index* $i_1 \ldots i_k$ is $S_{i_1\ldots i_k} = \frac{D_{i_1\ldots i_k}}{D}$. Note that the sum of the sensitivity indices is equal to one, since the functions $f_{i_1\ldots i_k}$ are orthogonal.

The first order indices have a natural probabilistic interpretation. It is easy to see that $f_i(x_i)$ equals the function $E(f|x_i) - f_0$. Hence we have that $D_i = \mathrm{Var}_{x_i}[E(f|x_i)]$. Now, since

$$\mathrm{Var}(f) = E_{x_i}\{\mathrm{Var}_{x_i}(f|x_i)\} + \mathrm{Var}_{x_i}[E(f|x_i)]$$

we see that D_i can be interpreted as the expected amount of variance reduction that would be achieved for f if we were able to specify x_i exactly.

Therefore, when the input variables are independent, the first order Sobol indices have two interpretations:

1. The uncertainty contribution of each variable to the overall variance;

2. The quality of the approximation made when f is approximated by the first order terms of the Sobol series expansion.

From the second interpretation, we see that "sensitivity with respect to a variable" can be defined in terms of the variance contribution of a function of only that variable in a series expansion of the original function. The problem with generalising this approach is however that there are various ways of generalising the Sobol series expansion when we are dealing with dependent variables.

3 TWO METHODS FOR EXPANDING FUNCTIONS WITH DEPENDENT VARIABLES

We consider the kinds of expansions into functions of different dimensions that might be possible for dependent variables. For convenience we assume that the function f has zero mean.

To motivate the different methods that we discuss consider first the Sobol expansion again. From a probabilistic point of view, a natural way of defining functions of different dimensions is to take conditional expectations. This gives a family of functions of the form

$$(x_{i_1}, \ldots, x_{i_k}) \mapsto E(f|x_{i_1} \ldots x_{i_k}) \tag{1}$$

for different $i_1 \ldots i_k$. One way of obtaining the Sobol expansion is to orthogonalise this family of functions. (Orthogonalisation is necessary to be able to decompose the variance). The orthogonalisation is quite straightforward, as all of the first order functions are already mutually orthogonal. The orthogonalisation of the second order functions is done by subtracting the corresponding first-order functions, for example

$$E(f|x_1, x_2) \text{ is transformed to } E(f|x_1, x_2) - E(f|x_1) - E(f|x_2).$$

Proceeding in this way, we see that the Gram-Schmidt orthogonalisation procedure applied to the functions in (1) (ordered lexicographically) gives the orthogonal family used in the Sobol expansion.

3.1 Orthogonalisation

In the case of dependent parameters, we can follow the procedure described above. This means that we take the functions in (1), ordered in some way (eg lexicographically) and apply the orthogonalisation procedure. Then, since f is in the linear space spanned by these functions, we can express it in a unique way as a linear combination of the orthgonalised functions.

Concretely, suppose the functions in (1) are have been ordered and are called $\tilde{g}_1, \ldots \tilde{g}_m$. They are orthogonalised inductively to give an orthogonal collection $g_1, \ldots, g_m$, defined by $g_1 = \tilde{g}_1$, $g_2 = \tilde{g}_2 - [\mathrm{Cov}(g_1, \tilde{g}_2)/\mathrm{Var}(g_1)] \cdot g_1 \ldots$ and in general,

$$g_k = \tilde{g}_k - \sum_{j=1}^{k-1} \frac{\mathrm{Cov}(g_j, \tilde{g}_k)}{\mathrm{Var}(g_j)} \cdot g_j.$$

We can now write $f = \sum[\mathrm{Cov}(f, g_i)/\mathrm{Var}(g_i)]g_i$, and, by rearranging the terms have f as a linear combination of the original functions $\tilde{g}_i$. Since the g_i's are orthogonal we also have a decomposition of the variance of f,

$$\mathrm{Var}(f) = \sum \frac{\mathrm{Cov}(f, g_i)^2}{\mathrm{Var}(g_i)}.$$

Furthermore, since each g_k is a linear combination of the $\tilde{g}_i$ with $i \leq k$, we see that the partial variances

$$\sum_{i=1}^{k} \frac{\mathrm{Cov}(f, g_i)^2}{\mathrm{Var}(g_i)}$$

tell us the degree of uncertainty of f accounted for in the first k terms. The term

$$\frac{\mathrm{Cov}(f, g_k)^2}{\mathrm{Var}(g_k)}$$

tells us how much extra uncertainty we can account for by making use of the kth term, when we have already used terms $1 \ldots k-1$.

It is important to realise that the uncertainty contributions calculated in this way are dependent upon the ordering of the functions in (1).

One heuristic is to order the first order terms $E(f|x_i)$ according to the size of their variances C_i, with the largest first. This however will not take into account the fact that the variances of two terms $E(f|x_i)$ and $E(f|x_j)$ could both be high if x_i and x_j are highly coupled.

3.2 Building a series by conditional expectations

An alternative way of constructing the functions in the Sobol series expansion in the case of independent variables is as follows. We define inductively $g_1 = E(f|x_1)$, $g_2 = E(f - g_1|x_2)$, $g_3 = E(f - g_1 - g_2|x_3) \ldots$ This gives a family of functions which is not the same as that in (1), unless the variables are independent. Furthermore this family is not orthogonal, and must be orthogonalised as above. We can then define uncertainty contributions as above. The uncertainty contributions are again dependent on the ordering of the variables.

3.3 Calculating the indices by MC simulation

The indices are not useful if one has to calculate the whole functional decomposition first. Fortunately the indices can be estimated in a Monte Carlo simulation in a similar fashion to the Sobol indices for independent variables.

In the dependent case however, we have to compute integrals with respect to rather complicated probability distributions. In general it will be difficult to simulate these distributions. When the distribution of the parameters $x_1 \ldots x_n$ has the form of a tree-dependent distribution (as are used by UNICORN, an uncertainty analysis code of the TU Delft [2]), it transpires that the more complicated distributions required for calculating the first order sensitivity indices are then also tree-dependent distributions. This means that simulation is straightforward.

As an example we show how the covariance of $f_1(x_1) = E(f|x_1)$ and $f_2(x_2) = E(f|x_2)$ can be calculated. Note that

$$\begin{aligned}
\mathrm{Cov}(f_1, f_2) &= E(f_1 f_2) \\
&= \int f_1(x_1) f_2(x_2) p(x_1, x_2, \ldots, x_n)\, dx_1 \ldots dx_n \\
&= \int\int f(x_1, \ldots, x_n) p(x_2, \ldots, x_n|x_1) \frac{d\underline{x}}{dx_1} \int f(x_1, \ldots, x_n) p(x_1, x_3, \ldots, x_n|x_2) \frac{d\underline{x}}{dx_2} p(\underline{x})\, d\underline{x}
\end{aligned}$$

where $d\underline{x} = dx_1 \ldots dx_n$ and $\frac{dx}{dx_1} = dx_2 \ldots dx_n$, etc.. Introducing new variables $\underline{u} = (u_2, \ldots, u_n)$ and $v = (v_1, v_3, \ldots, v_n)$, we can write the last expression above as

$$\begin{aligned}
&\int\int f(x_1, u_2 \ldots, u_n) p(u_2, \ldots, u_n|x_1)\, d\underline{u} \int f(v_1, x_2, v_3, \ldots, v_n) p(v_1, v_3, \ldots, v_n|x_2)\, d\underline{v} p(x_1, x_2)\, dx_1\, dx_2 \\
= &\int f(x_1, u_2 \ldots, u_n) f(v_1, x_2, v_3, \ldots, v_n) p(u_2, \ldots, u_n|x_1) p(v_1, v_3, \ldots, v_n|x_2) p(x_1, x_2)\, d\underline{u}\, d\underline{v}\, dx_1\, dx_2.
\end{aligned}$$

Hence the covariance is obtained by integrating the function $f(x_1, u_2 \ldots, u_n) f(v_1, x_2, v_3, \ldots, v_n)$ with the probability density

$$p(u_2, \ldots, u_n|x_1) p(v_1, v_3, \ldots, v_n|x_2) p(x_1, x_2).$$

Suppose that the probability density of the original variables was a tree dependent density as shown in Figure 1.
Then the density for the variables $\underline{u}$, $\underline{v}$, x_1 and x_2 is also tree dependent with tree shown in Figure 2.

4 CONCLUSION

We have shown that the sensitivity indices defined by Sobol for independent variables can be generalised in two ways for dependent variables. These ways are associated with a series expansion of the function, and the values taken by the indices depend on the ordering of the variables.

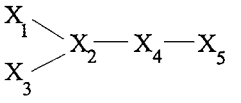

Figure 1: Tree dependent variables

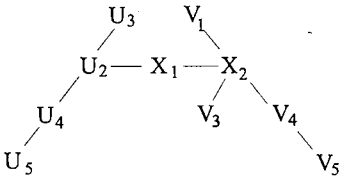

Figure 2: More tree dependent variables

When the variables are tree-dependent then the indices can be calculated by Monte Carlo simulation of various tree-dependent distributions.

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SENSITIVITY COEFFICIENTS IN CHARGED PARTICLE OPTICS

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1 INTRODUCTION

Charge Particle Optics deals with the beams of charged particles (electrons, ions and sometimes dipole molecules) which move in some space with electric and magnetic fields. In most cases the fields under consideration are time independent (i.e., electrostatic and magnetostatic fields), and the beam is weak enough to neglect the space charge and space currents induced by the beam itself. The corresponding mathematical problem seems to be trivial (the Newton's equations of movement in specified external field) except the fact that the devices based on Charged Particle Optics [1] play an important role in modern science.

The sensitivity is an important and complex problem in Charged Particle Optics (like that in each manufacturing). There are two important aspects of this problem:

- how the manufacturing errors influence the field inaccuracies,
- how the field inaccuracies influence the beam properties.

There are many ways how to specify and to solve these principal problems. This paper considers the following aspects:

- how to calculate at any point the field sensitivity to small variations of the electrodes using the boundary element method,
- how to calculate the parasitic aberrations of the beam caused by the field sensitivity to some external variations.

Both algorithms should be extremely useful in numerical calculations in Charged Particle Optics.

2 BOUNDARY ELEMENT METHOD AND VARIATIONS

The algorithm considered in this section follows the idea suggested by M.A.Monastyrsky [3] which associates the field variations caused by imperfect electrodes with some parasitic charges distributed along the ideal electrodes. It assumes essentially that the field is calculated using the Boundary Element Method [2] (i.e., as the integral over the electrodes of some charge density). It will be shown that the field variations caused by the variations of the electrodes and the boundary conditions can be represented as well like the integrals of some variational charge density over the same electrodes, although in this case the integral kernel ("potential of a point charge"), boundary conditions and the variational "charge density" do not have such direct physical interpretation.

Consider as an example the two-dimensional Laplace equation with Dirichet boundary conditions $U_{xx} + U_{yy} = 0$, $U|_{\Gamma_k} = f_k(s)$ Using the Boundary Element Method the field is represented as the integral over the electrodes:

$$U(x,y) = \sum_j \int_{\Gamma_j} \rho_j(s) K_j(s,x,y)\, ds \tag{1}$$

where $\Gamma_j = \{x_j(s), y_j(s), s \in [s_j^a, s_j^b]\}$ are the boundaries (electrodes), the integral kernels are the potentials of a point charge: $K_j(s,x,y) = K(x_j,y_j,x,y) = \log\left((x_j(s)-x)^2 + (y_j(s)-y)^2\right)$, and

$\rho_j(s)$ are the unknown charge distributions along the electrodes. If we substitute in (1) the value $(x_k^+, y_k^+) = (x_k(s_k^+), y_k(s_k^+))$ (the point selected at the boundary Γ_k) the resulting integral equation

$$\sum_j \int_{\Gamma_j} \rho_j(s) K_j(s, x_k^+, y_k^+)\, ds = f_k(s_k^+) \tag{2}$$

enables to calculate the unknown charges $\rho_j(s)$.

Suppose that the boundary conditions and the boundaries itself are variated, so that the right hand side functions $f_k^*(\alpha, s)$, the boundaries $\Gamma_k^* = \{x_k^*(\alpha, s^*), y_k^*(\alpha, s^*), s \in [s_k^a, s_k^b]\}$ and the charge distributions $\rho_k^*(s^*)$ are substituted in (1)–(2) (here α is some "small parameter"of variation). The parametrizations of Γ_k and Γ_k^* are related as $s^* = \varphi_k(\alpha, s)$. For small α

$$\begin{array}{ll} x_k^*(\alpha, s^*) = x_k(s) + \alpha X_k(s) + \ldots, & y_k^*(\alpha, s^*) = y_k(s) + \alpha Y_k(s) + \ldots, \\ f_k^*(\alpha, s^*) = f_k(s) + \alpha F_k(s) + \ldots, & \rho_k^*(\alpha, s^*) = \rho_k(s) + \alpha R_k(s) + \ldots, \\ s_k^*(\alpha, s) = s + \alpha S_k(s) + \ldots, & \end{array} \tag{3}$$

The variation of the solution $U^*(x,y) - U(x,y) \approx \alpha V(x,y) + \ldots$ induced by this variation of the boundary conditions is given by the following expression derived from (1):

$$\begin{aligned} V(x,y) = & \sum_j \int_{\Gamma_j} \left(R_j + \frac{\partial \rho_j}{\partial s} S_j + 2\rho_j \frac{\partial S_j}{\partial s} \right) K_j\, ds \\ & + \sum_j \int_{\Gamma_j} \rho_j \left(\frac{\partial K_j}{\partial x_j} \left(X_j + \frac{\partial x_j}{\partial s} S_j \right) + \frac{\partial K_j}{\partial y_j} \left(Y_j + \frac{\partial y_j}{\partial s} S_j \right) \right) ds \end{aligned} \tag{4}$$

where $K_j = K(x_j, y_j, x, y) = K(x_j(s), y_j(s), x, y)$. The variational charge density $R_k(s)$ (which is the only unknown value in (4)) is calculated through the integral equation derived from (4) in a way similar to deriving (2) from (1) and the boundary conditions.

This base idea enables to calculate at any point and with high accuracy the field variation induced by the electrode and potential variation. It can be extended in several ways. The obvious way is to apply it to other type partial differential equations which enable the representation of the solution through some boundary elements. The other way is to consider high order variational terms and the multiparameter $(\alpha, \beta, \gamma, \ldots)$ variations so that non-linear effects could be taken into account. Finally, it is possible to use alternative boundary element representations like [4] to get better accuracy near the boundaries and especially near the end points of the boundaries.

The numerical realizations of corresponding algorithms require more efforts than it can be viewed from the formula (4). Since the integral kernels become singular at the boundary, it is necessary to eliminate these singularities carefully before solving the integral equation and calculating the variation of the solution. The higher is the order of variational term, the greater is the order of singularity and the greater are the efforts necessary to eliminate it.

3 PARASITIC ABERRATION COEFFICIENTS

In Charged Particle Optics the behaviour of the trajectories of charged particles in electrostatic and magnetic fields are often described with the help of aberration coefficients [1, 5]. The aberration coefficients describe the deviation of the trajectory with respect to the base trajectory of the beam as a restricted Taylor set through the variations of the initial parameters x, y, a, b, μ, ϵ of the charged particle (see [1, 5] for more details):

$$\begin{aligned} X &= \langle \mathrm{X}| + \langle \mathrm{X}|\mathrm{x}\rangle x + \langle \mathrm{X}|\mathrm{y}\rangle y + \langle \mathrm{X}|\mathrm{a}\rangle a + \ldots + \langle \mathrm{X}|\mathrm{xx}\rangle x^2 + \langle \mathrm{X}|\mathrm{xy}\rangle xy + \\ &\quad + \langle \mathrm{X}|\mathrm{xa}\rangle xa + \ldots + \langle \mathrm{X}|\mathrm{yy}\rangle y^2 + \langle \mathrm{X}|\mathrm{ya}\rangle ya \ldots + \langle \mathrm{X}|\mathrm{xxx}\rangle x^3 + \ldots \\ Y &= \langle \mathrm{Y}| + \langle \mathrm{Y}|\mathrm{x}\rangle x + \langle \mathrm{Y}|\mathrm{y}\rangle y + \langle \mathrm{Y}|\mathrm{a}\rangle a + \ldots + \langle \mathrm{Y}|\mathrm{xx}\rangle x^2 + \langle \mathrm{Y}|\mathrm{xy}\rangle xy + \\ &\quad + \langle \mathrm{Y}|\mathrm{xa}\rangle xa + \ldots + \langle \mathrm{Y}|\mathrm{yy}\rangle y^2 + \langle \mathrm{Y}|\mathrm{ya}\rangle ya \ldots + \langle \mathrm{Y}|\mathrm{xxx}\rangle x^3 + \ldots \\ A &= \langle \mathrm{A}| + \langle \mathrm{A}|\mathrm{x}\rangle x + \langle \mathrm{A}|\mathrm{y}\rangle y + \langle \mathrm{A}|\mathrm{a}\rangle a + \ldots + \langle \mathrm{A}|\mathrm{xx}\rangle x^2 + \langle \mathrm{A}|\mathrm{xy}\rangle xy + \\ &\quad + \langle \mathrm{A}|\mathrm{xa}\rangle xa + \ldots + \langle \mathrm{A}|\mathrm{yy}\rangle y^2 + \langle \mathrm{A}|\mathrm{ya}\rangle ya \ldots + \langle \mathrm{A}|\mathrm{xxx}\rangle x^3 + \ldots \\ &\ldots \end{aligned} \tag{5}$$

The linear terms describe the ideal properties of the Gaussian optics, and hign order terms describe non-linear distortions of the image. Generally the derivation of the analytical expressions for aberration coefficients requires sophisticated mathematical techniques and a lot of human and computer time [5]. There are also several numerical approaches like [6] which enable to calculate the aberration coefficients with high accuracy provided that the external field is known precisely with its high order derivatives.

Except the variations of the trajectories caused by the variations of the initial conditions there are that caused by the variations of the external field. The latter are caused by the small variations (imperfections, manufacturing errors, etc.) of the electrode configurations, potentials and currents used to exite the electrostatic and magnetostatic fields, etc., and their analysis is essential in designing the corresponding devices.

To calculate the parasitic aberrations caused by the field variations considered in the previous section the generalization of the algorithm [6] is used. It enables to calculate numerically such variations of the trajectories provided that the field variations are already known.

Suppose that the external field is a function of some parameter which is considered as the parameter of variation. As a result the trajectiry equations have a form

$$\left\{ \begin{array}{rcl} X_k'(t) & = & F_k(X_1, X_2, \ldots, t, \alpha, \beta, \ldots) \\ X_k(0) & = & X_k^0 \end{array} \right. \tag{6}$$

where $(\alpha, \beta, \ldots)$ are the variations of the external field. The aberration representation (5) becomes the function of the variation which means that the aberration coefficients themselves can be represented as the restricted Taylor sets:

$$\left\{ \begin{array}{l} \langle \mathrm{X}| \rangle = [\mathrm{X}|] + [\mathrm{X}|\alpha]\,\alpha + [\mathrm{X}|\beta]\,\beta + \ldots + \left[\mathrm{X}|\alpha^2\right]\alpha^2 + \ldots \\ \langle \mathrm{X}|\mathrm{x} \rangle = [\mathrm{X}|\mathrm{x}] + [\mathrm{X}|\mathrm{x}\alpha]\,\alpha + [\mathrm{X}|\mathrm{x}\beta]\,\beta + \ldots + \left[\mathrm{X}|\mathrm{x}\alpha^2\right]\alpha^2 + \ldots \\ \langle \mathrm{X}|\mathrm{xa} \rangle = [\mathrm{X}|\mathrm{xa}] + [\mathrm{X}|\mathrm{xa}\alpha]\,\alpha + [\mathrm{X}|\mathrm{xa}\beta]\,\beta + \ldots + \left[\mathrm{X}|\mathrm{xa}\alpha^2\right]\alpha^2 + \ldots \\ \ldots \end{array} \right. \tag{7}$$

The Taylor set coefficients (i.e., the aberration coefficients in (5) and (7)) are actually the defivarives of the trajectory function $X(t, x, y, a, \ldots, \alpha, \beta, \ldots)$ with respect to the variation parameters. To calculate their values directly from the system of differential equations (6) we should *differentiate* the right hand side and the left hand side functions of (6) with respect to $x, y, a, \ldots, \alpha, \beta, \ldots$. It results to the *extended system* of trajectory differential equations:

$$\left\{ \begin{array}{rcl} X_k' & = & F_k \\ \left(\dfrac{\partial X_k}{\partial \varepsilon_p}\right)' & = & \dfrac{\partial F_k}{\partial \varepsilon_p} + \displaystyle\sum_i \frac{\partial F_k}{\partial X_i}\frac{\partial X_i}{\partial \varepsilon_p} \\ \left(\dfrac{\partial^2 X_k}{\partial \varepsilon_p \partial \varepsilon_q}\right)' & = & \dfrac{\partial^2 F_k}{\partial \varepsilon_p \partial \varepsilon_q} + \displaystyle\sum_i \frac{\partial F_k}{\partial X_i}\frac{\partial^2 X_i}{\partial \varepsilon_p \partial \varepsilon_q} + \sum_{i,j} \frac{\partial^2 F_k}{\partial X_i \partial X_j}\frac{\partial X_i}{\partial \varepsilon_p}\frac{\partial X_j}{\partial \varepsilon_q} \\ & & \quad + \displaystyle\sum_i \left(\frac{\partial^2 F_k}{\partial X_i \partial \varepsilon_p}\frac{\partial X_i}{\partial \varepsilon_q} + \frac{\partial^2 F_k}{\partial X_i \partial \varepsilon_q}\frac{\partial X_i}{\partial \varepsilon_p} \right) \\ \ldots \end{array} \right. \tag{8}$$

where $(\varepsilon_p, \varepsilon_q,)$ stand for the variations of the initial conditions $(x, y, a, \ldots)$ and the field variation $(\alpha, \beta, \ldots)$ as well. The unknown functions

$$\frac{\partial X_k}{\partial x}, \frac{\partial X_k}{\partial a}, \frac{\partial X_k}{\partial \alpha}, \frac{\partial^2 X_k}{\partial x^2}, \frac{\partial^2 X_k}{\partial x \partial a}, \frac{\partial^2 X_k}{\partial y \partial \beta}, \frac{\partial^2 X_k}{\partial \alpha^2}, \ldots$$

stands for the aberration coefficients. To solve the system (8) numerically it is necessary to add the initial conditions

$$\left\{ \begin{array}{llllll} \left.\dfrac{\partial X}{\partial x}\right|_{t=0} = 1, & \left.\dfrac{\partial X}{\partial y}\right|_{t=0} = 0, & \left.\dfrac{\partial X}{\partial a}\right|_{t=0} = 0, & \left.\dfrac{\partial X}{\partial \beta}\right|_{t=0} = 0, & \ldots \\ \left.\dfrac{\partial^2 X}{\partial x^2}\right|_{t=0} = 0, & \left.\dfrac{\partial^2 X}{\partial x \partial y}\right|_{t=0} = 0, & \left.\dfrac{\partial^2 X}{\partial x \partial \beta}\right|_{t=0} = 0, & \left.\dfrac{\partial^2 X}{\partial^2 \beta}\right|_{t=0} = 0, & \ldots \end{array} \right. \tag{9}$$

specific to the aberration coefficients. The parallel numerical integration of (8) together with (9) gives the base trajectory of the beam and the full set of the aberration coefficients at each trajectory point (although generally we are interested in aberration coefficients at the final point of the trajectory only).

4 CONCLUSION

It is shown that it is possible to calculate in one step the "canonical" aberrations caused by the variations of the initial conditions and the "imperfect" aberrations (or sensitivity coefficients) caused by the variations of the geometry of the electrodes and their potentials. To do it (i.e., to solve (8)–(9) numerically) it is necessary to know with high precision the high order derivatives of the field and the field sensitivity coefficients at each point of the base trajectory or at each point of the beam region if the base trajectory is not known in advance. The boundary element method when used for field calculations enables to calculate with high accuracy the high order derivatives of the field. The modification of the boundary element method considered here enables to calculate the high order field sensitivity coefficients parallelly to the field calculation. It is essential that the high order field derivatives, high order variational coefficients and the high order derivatives of variational coefficients can calculated with the uniformly high precision since all differentiations are performed analytically inside integral formulae. To achieve in practice for numerical calculations high accuracy requires some special refinements of the numerical algorithm (first of all, special treatment of numerical integration for the *singular* integral kernels with good accuracy up to the boundary of the integration). Unfortunately, the detailed consideration of these pecularities does not fit to the size of this short abstract.

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EQUIFINALITY AS A BASIS FOR UNCERTAINTY ESTIMATION IN ENVIRONMENTAL MODELLING

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ABSTRACT

The available models for most environmental systems are not very good. There are, however, many good reasons for this, including lack of knowledge of the controlling processes, lack of appropriate descriptive theories at the scales at which predictions area required, errors in initial and boundary conditions (often with nonstationary statistical structure), errors in input forcing data and calibration data, the difficulties of measuring the complex characteristics of the system of interest and the limitations of numerical algorithms and computational power. One result is that in many areas of environmental modelling there are no commonly agreed modelling strategies but rather many competing models. Thus, although environmental systems are complex and cannot or cannot easily be controlled for experimental purposes, the problem is not usually that there is a lack of available models, since even in data scarce situations, models are still commonly constructed for quantitative prediction. The problem is rather that there are too many models available, all of which work (at least if some calibration or flux adjustments are allowed) and all of which are known to be wrong (though as modellers we tend not to talk about that too much, but see the analysis of Morton, 1993).

Experience with a variety of hydrological and geochemical models has revealed that errors in inputs, observed outputs and model structure do not generally result in a well defined optimum parameter set but in a large number of different model structures and parameter sets within model structures that are acceptably consistent with the calibration data. This has been called the equifinality problem by Beven (1993, 1996a,b). The term equifinality has been chosen deliberately (rather than non-identifiability or model structural uncertainty) to focus attention on the many models that might be considered acceptable and on the rejection of the concept of an optimal model. A Monte Carlo simulation methodology (Generalised Likelihood Uncertainty Estimation, GLUE) has been developed as a way of proceeding with uncertainty estimation for predictions in the face of equifinality (see Beven and Binley, 1992). It is an example of the wider class of uncertainty estimation methodologies discussed by Klir (1994). The methodology is consistent with Bayesian techniques but allows a wider range of (subjective) likelihood measures and fuzzy measures to be used in uncertainty estimation. The methodology focuses attention on the value of different types of data in model rejection and conditioning uncertainty estimates.

The elements of the GLUE methodology are as follows (Beven and Binley, 1992):

- a prior (subjective) choice of parameter distributions
- a procedure for sampling random values of the parameters
- a (subjective) choice of likelihood measure to evaluate the performance of each parameter set in the model with respect to some calibration data (which may also be qualitative as well as quantitative)
- a procedure for quantifying uncertainty in the nonlinear model simulations, in the form of prediction quantiles for different variables of interest, given the likelihood values for each parameter set
- procedures for updating the likelihoods associated with each parameter set as new calibration data becomes available (Bayes equation can be used but there are other possibilities) and evaluating the worth of additional data in constraining the predictive uncertainty

An important feature of the GLUE approach is that the likelihood measures are associated with the sets of parameter values. All effects of interaction and correlation between parameters are therefore included implicitly within the likelihood values in so far as such effects are important to the functional performance of the model in reproducing the calibration data. Sensitivity of the model results with respect to the individual parameters is not, therefore, necessarily meaningful but can be evaluated by calculating the marginal distributions for parameters in different model functional classes (essentially a generalised form of the Regionalised Sensitivity Analysis of Hornberger and Spear, 1981). Likelihood values are explicitly conditional on the model structure, parameter set, and input and output data sequences used. Multiple model structures can be considered within the same framework subject to the constraint that all models can be assessed using the same likelihood measures.

An important constraint of the GLUE approach is that, for high dimensional models, computational limitations become important in fully evaluating the likelihood surface. In most example applications that we have examined, the structure of the likelihood surface has been such that some form of importance sampling strategy would not be greatly advantageous, acceptable simulations tend to be found across the sampled ranges of most parameters and uniform sampling has generally been used (examples will be given). The simulations are also readily implemented on distributed memory parallel machines (such as the Lancaster PARAMID system) or networks of distributed workstations using PVM.

The GLUE methodology has now been applied to a variety of applications including rainfall-runoff modelling (e.g. Beven and Binley, 1992; Beven, 1993; Romanowicz et al., 1994, Freer et al., 1996; Franks et al., 1997), modelling contaminant transport in groundwaters (Buckley et al., 1995), modelling flood inundation (Romanowicz and Beven, 1996,1997), modelling land surface to atmosphere fluxes (Franks et al., 1997), and modelling soil geochemistry (Zak et al., 1997). A demonstration PC program to illustrate the concepts can be downloaded from the World Wide Web at http://www.es.lancs.ac.uk/es/Freeware/Freeware.html.

This presentation will concentrate on the evaluation of change in a hydrological system within an equifinality framework. It will be shown how the effects of a major forest fire on the hydrology of a small Mediterranean catchment can be followed in terms of the changing parameter distributions in the period of recovery after the fire, despite the uncertainty associated with the model predictions. This is one example of a model of the response of an environmental system must be inherently uncertain. The data available do not allow a clear unequivocal representation of the process response of the catchment before the fire, while the effects of the fire are likely to have had an impact on the catchment characteristics, particularly those of the near surface soil in a way that may change the processes by which the catchment responds to rainstorms. This study has made use of a version of the rainfall-runoff model TOPMODEL, which uses simplified physical theory to describe runoff generation processes (see for example Beven et al., 1996; Beven, 1997). A more complete, but also parametrically more complex, physical representation of this same catchment has been provided by an application of the *Système Hydrologique Européen* (SHE) model (Parkin et al., 1996). The SHE application demonstrates the range of predictions that may result from physically feasible parameter ranges in this environment.

In this study we have used 5 different periods of hydrological data, before and after the fire to condition 10,000 randomly chosen parameter sets within the GLUE framework using different likelihood measures. The results of individual periods of conditioning demonstrate the many different parameter sets that are consistent with the data, at least to within the limits of predictability inherent in the use of the TOPMODEL structure and the observations being used in the conditioning. Likelihood weighted predictions are used to demonstrate the predictive uncertainty of the model. Subdividing the parameter sets for each period on the basis of their functionality in reproducing the observations, shows that the class with the highest likelihood values shows a strong response to the fire for certain parameters. There is then a recovery in these parameter distributions during the period of regrowth after the fire.

One of the issues in environmental modelling is whether predictions of the impacts of changed conditions are significant in comparison with the uncertainty of predictions assuming no change (e.g. Binley et al., 1991). In this particular example, it appears that the extreme effects of fire on this catchment do allow changes in some parameter values to be distinguished, despite the high uncertainty of the modelling. However, it should be noted in conclusion that here the data are being used to constrain the feasible parameter sets through and that it is a very different matter to make estimates of what feasible parameter sets might be prior to a change taking place.

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SENSITIVITY ANALYSIS OF A CGE MODEL FOR POLAND

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1 INTRODUCTION

Computable General Equilibrium (CGE) models have become a wide-spread scientific tool with a steadily increasing importance for policy debate on tax issues.

A new CGE model for Poland and a tool for sensitivity analysis are presented. The goal of building the model is to investigate macroeconomic processes in the market economy.

CGE models are by far the most developed models that attempt to derive quantitative economy-wide implications of the interdependence of micro-economic actors. These models have been successfully applied in many countries, especially in the areas of tax policy and international trade[1-3].

The following features of CGE models stand out:

- CGE models are economy wide, taking into account direct and indirect effects of exogenous changes on producers in different industries and household in different socio-economic groups.
- Modeling of economic behavior has a firm theoretical foundation, which enables the generation of results in circumstances for which there is no historical experience.
- The Constant Elasticity of Substitution-Constant Elasticity of Transformation (CES-CET) specification of technology employed in CGE models provide an exact and theoretically consistent measure of producer gains to research.

Policy simulation can be performed by changing tax rates or other policy instruments. A new equilibrium (counterfactual equilibrium) is calculated for each policy change. Policy decisions are derived by comparing the endogenous variables in the counterfactual equilibrium with those of the benchmark equilibrium.

Decision analysis can be used in conjunction with the model and with other analytic techniques including sensitivity analyses. Decision analysis provides measures of the benefits that can potentially be achieved by making changes to the input (taxes, prices, production technologies, expectations).

A tool for the investigation of the model sensitivity analysis is a special program that generates input parameter values, solves an optimization task that includes equations of the model and a goal function and transforms solutions to a desired form.

2 A CGE MODEL

A CGE model for Poland was built on the base of Poland's national account date. The model can be used to evaluate economic policies in international trade, taxation, planning government budget.

The following conditions hold for this model:

- demands equal supplies for goods and factors;
- all domestic agents satisfy their budget constraints;
- government satisfies its budget constrains;
- producer behavior is characterized by cost minimization for a given output.

The model consists of the following blocks: prices, budget income, government expenditure and budget constraints, productive technology, income generation, consumption and savings, investment and stock changes, export demand, market clearing requirements, and objective functions. Each block is a set of nonlinear algebraic equations. The model has about 80 equations[4].

The model takes into account approximately 120 variables and 50 parameters. Some of these variables are: composite output, domestic production, gross output, domestic sales, export, final import demands, value added, intermediate goods, capital stock, employment of wage labor, various prices. Some of the important parameters are: international prices, import prices by commodity, exchange rate, scaling for production functions, scaling for CET- function, share parameter for CET-function, Armington- function exponent, depreciation rate for capital income, scaling for export demand function, elasticity of transformation, elasticity of substitution.

3 MODEL IMPLEMENTATION

The model is implemented as a program in GAMS(General Algebraic Modeling System), providing a high-level computer language for the compact presentation of large and complex models, allowing changes to be made in model specifications simply and safely, and permitting model descriptions that are independent of solution algorithms[5]. GAMS is specifically designed for modeling linear, nonlinear, and mixed integer optimization problems. The system is especially useful with large, complex models. GAMS is available for use on personal computers, workstations, main-frames, and supercomputers. GAMS lets the user concentrate on modeling, eliminating the need to think about purely technical, machine-specific problems.

The program consists of (i) the calibration block, (ii) the block representing equations of the model, and (iii) the block that transforms results and forms them as a desired structure.

The calibration is the procedure to determine parameter values such as to exactly reproduce the adjust data set of the base year. The usual practice is to borrow a sufficient number of extraneous estimates of elasticities from the econometric literature. The remaining parameter values are determined in a nonstochastic manner by solving each agent's equilibrium conditions for parameters in question using the data on prices and quantities in the benchmark equilibrium data set. The estimates of elastisities are not very reliable, so we need to perform some sensitivity analyses.

The calibration of the model was carried out for Poland's national accounts data for 1994.

4 A TECHNIQUE AND A TOOL FOR SENSITIVITY ANALYSIS

Calculating multipliers was chosen as a basic technique for carrying out sensitivity analysis of the output, i.e. calculating the changes in the endogenous variables in response to those in elasticities and taxes. Since our model is nonlinear we need to compute multipliers by means of numerical simulation of the model as the ratio of the changes in the endogenous variable with respect to changes in elasticities and taxes. The computation of multipliers involves two solutions of the model: the control solution and the disturbed solution, i.e. solution when an increment is given to level of the some elasticity or tax.

A program in the GAMS language was built to provide measures of the changes in the output of the model that are attributable to changes in the input. The program permits to choose any parameter and determine an interval in which the parameter can be vary [parmin, parmax]. Next the program forms (n+1) values of the parameter: parmin, parmin+h, parmin+2h,..., parmax; where h=(parmax-parmin)/n and solves the model for each value. Results of the program are formed in the form of a table that can be used for the following analyses by a GAMS program or by standard tools(EXEL, C, FORTRAN). For example, multipliers, i.e. the changes in the endogenous(output) variables in response to those in chosen exogenous(input) variables can be easily computed by means of analytical formulae written in GAMS, C, FORTRAN, or other languages.

5 RESULTS OF SENSITIVITY ANALYSIS

Presently the authors investigate how tax policy changes affect Polish macroeconomy indicators. The authors have used the program to study how the following variables: composite output, domestic production, gross output, domestic sales, export, final import demands, value added intermediate goods, household consumption, total gross investments, gross enterprise income, total government income, domestic final demand, household savings, and various prices depend on the following input parameters :

1) export elasticity;
2) elasticity of substitution between domestic sales and import;
3) elasticity of transformation between export and domestic sales;
4) elasticity of substitution between value added and intermediate goods;
5) elasticity of substitution between capital stock and employment of wage labor.

Tax policies were simulated by the study of sensitivity analysis of the model output in dependence on the following tax rates:

1) import tax rate;
2) tax rate on wage;
3) tax rate on excise goods;
4) tax rate on enterprise income;
5) tax rate on final demand;
6) tax rate on indirect taxes.

Results of the sensitivity analysis are a set of multipliers - the changes in the mentioned endogenous variables in response to those in elasticities and tax rates as well as a set of curves that were built on the base of the tables generated by means of the program for sensitivity analysis. Each curve represents a dependence of a macroeconomic indicator upon one of the mentioned input parameters.

6 CONCLUSION

The CGE model and the tool for sensitivity analysis are strong in analyzing the allocation of production factors to alternative uses. The analysis in the CGE model investigates optimal responses of producers and consumers to changes in prices, imposing consistency between the firm's beliefs about prices and their equilibrium realization. Through general equilibrium and sensitivity analyses it becomes possible to judge the full effects of policy changes. Another advantage of the model is its flexibility to incorporate alternative behavioral specifications. Through this feature such a model can be used as a testing ground for competing theoretical assumptions, including typical General Equilibrium assumptions. The implementation of the model as a GAMS program permits to solve not only the equations of the model, but also to solve various optimization tasks that policy makers formulate.

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AUTOMATIC DIFFERENTIATION — PRINCIPLES, TOOLS, AND APPLICATIONS IN SENSITIVITY ANALYSIS

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1 INTRODUCTION

Let f be a computer model, and denote by $f(x)$ the output it produces for a particular input x. Employing the Taylor expansion of f around a reference state x_o, we have

$$f(x_o + \Delta x) = f(x_o) + \frac{\partial f(x_o)}{\partial x}\Delta x + HO(x_o, \Delta x),$$

where the higher-order terms $HO(x_o, \Delta x)$ satisfy $||HO(x_o, \Delta x)|| = O(||\Delta x||^2)$. Hence, the value of the first-order derivatives allows us to derive a linear first-order approximation of f around the base state x_o. Higher-order approximations of f can be derived by continuing the Taylor series further, e.g. 2nd order derivatives provide a quadratic model.

Thus, derivatives provide a way to compute a relatively simple approximation of f, and allow one to inexpensively explore the behavior of f in the neighborhood of x_o. One application of derivatives is in sensitivity analysis, where one tries, for example, to assess the sensitivity of a computational model to perturbations in its parameters or initial conditions to verify robustness with respect to empirically determined parameters or to verify that the model behaves as suggested by experimental data.

This paper focuses on the efficient and accurate computation of derivatives for arbitrary computer programs using a method called "automatic differentiation (AD)." While it is clear that derivative-based approaches to sensitivity analysis are not appropriate for all contexts, derivatives provide one mechanism for understanding the behavior of computer models, and the goal of our work is to facilitate this particular process. We motivate the principles behind AD and briefly highlight application projects in mesoscale weather modeling and atmospheric chemistry where AD was employed to assess the sensitivity of the model w.r.t. initial conditions and to help determine dominant chemical reactions.

2 AUTOMATIC DIFFERENTIATION

For purposes of illustration, assume that we have a code for the computation of a function f and $f : x \in \mathbf{R}^n \mapsto y \in \mathbf{R}^m$, and we wish to compute the derivatives of y with respect to x. Traditionally, derivatives have been computed in one of the following three ways:

By Hand: One can differentiate the code by hand and thus arrive at a code that also computes derivatives. Alternatively, one can mathematically derive expressions for derivatives, and then implement a program to compute them. However, handcoding of derivatives for a large code is a tedious and error-prone process.

Divided Differences: One can approximate the derivative of f with respect to the ith component of x at a particular point x_0 for example by *one-sided differences*

$$\left.\frac{\partial f(x)}{\partial x_i}\right|_{x=x_0} \approx \frac{f(x_0 \pm h * e_i) - f(x_0)}{\pm h}.$$

Here e_i is the ith Cartesian basis vector. This approach leads to a first-order approximation of the desired derivatives. Computing derivatives by divided differences has the advantage that we need only the function as a "black box," but their accuracy may be hard to assess.

Symbolic Differentiation: Symbolic manipulators like Maple, Macsyma, or Reduce provide powerful capabilities for manipulating algebraic expressions. However, their application to larger computer programs typically requires some human effort to break down the code into pieces and to assemble the resulting pieces into a usable derivative code.

In contrast, our work is based on a technique called *automatic differentiation*. Automatic differentiation techniques rely on the fact that every function, no matter how complicated, is executed on a computer as a (potentially very long) sequence of elementary operations such as additions, multiplications, and elementary functions such as `sin` and `cos`. By applying the chain rule of differential calculus, e.g.,

$$\frac{\partial}{\partial t} f(g(t))\Big|_{t=t_0} = \left(\frac{\partial}{\partial s} f(s)\Big|_{s=g(t_0)}\right)\left(\frac{\partial}{\partial t} g(t)\Big|_{t=t_0}\right)$$

over and over again to the composition of those elementary operations, one can compute, in a completely mechanical fashion, derivatives of f that are correct up to machine precision [1, 2]. The techniques of automatic differentiation are directly applicable to computer programs of arbitrary length containing branches, loops, and subroutines, and can be generalized to derivatives of arbitrary order.

2.1 The Forward Mode of AD

The most straightforward application of the fundamental idea underlying automatic differentiation leads to the so-called forward mode of automatic differentiation. Here we maintain derivatives of intermediate values with respect to input variables and propagate derivatives alongside the execution of the original program. We associate with each program variable x a gradient object ∇x to hold its associated derivative object and arrive at a code that computes

$$\nabla y[i] = \sum_{j=1,\ldots,n} \frac{d\, y[i]}{d\, x[j]} * \nabla x[j], i = 1, \ldots, m \tag{1}$$

Through proper choice of $\nabla x[j]$ we can thus compute a set of arbitrary directional derivatives, and the computation of one column of a Jacobian is just a special case. The computational complexity of the forward mode is proportional to the number of directional derivatives that we are computing.

2.2 The Reverse Mode

An alternative approach to the automatic computation of derivatives is the so-called reverse mode. Here, we propagate derivatives of program outputs with respect to intermediate values, and this type of derivatives is typically called an *adjoint*. To propagate adjoints, we need to be able to reverse the partial order of program execution. This implies, for example, that we need to remember which way a particular branch was taken. We also may need to store or recompute the value that a particular variable held at a given point in the program. In the reverse pass, we associate an adjoint object $\bar{\nabla}$ with every program variable, and update them according to an adjoint rule:

$$s = f(u, v) \Longrightarrow \begin{cases} \bar{\nabla} u = \bar{\nabla} u + \frac{\partial f}{\partial u} * \bar{\nabla} s; \\ \bar{\nabla} v = \bar{\nabla} v + \frac{\partial f}{\partial v} * \bar{\nabla} s; \end{cases} \tag{2}$$

In contrast to the forward mode, the reverse mode allows us to compute an arbitrary linear combination of rows of the Jacobian or, in particular, the gradient of a particular output variable with respect to all program inputs. In this particular case, the floating-point requirements of the code are at most five times that of the original code. The memory cost is more difficult to assess due to the need for storing intermediate values. In the worst case, it can be proportional to the number of floating-point operations

performed in the program. However, this is a pessimistic assumption, and actual memory requirements may be much less.

A detailed example of the forward and the reverse mode is presented in [3]. In addition to the forward and reverse mode, the associativity of the chain rule of differential calculus allows for many other ways of accumulating derivatives with rather different computational requirements. The development of improved AD algorithms is an area of active research (see, for example, the articles in [4, 5]).

3 AUTOMATIC DIFFERENTIATION TOOLS

Recently, there has been much progress in the development of tools that augment Fortran and C programs with statements for the computation of derivatives based on the principles of automatic differentiation. We are involved in the development of the ADIFOR/ADJIFOR and ADIC/ADJIC tools for Fortran 77 and ANSI-C codes, respectively. These tools are based on advanced compiler infrastructure and thus are able to deal with arbitrary computer programs, e.g., containing an arbitrary number of subroutines, or COMMON blocks and EQUIVALENCEs in Fortran, or pointers or arbitrary structures in C.

The ADIFOR (Automatic Differentiation of Fortran) [6, 3] tool, a joint project of Argonne National Laboratory and Rice University, has been under development for six years and is available at `http://www.mcs.anl.gov/adifor` and `http://www.cs.rice.edu/~adifor`. ADIFOR has been successfully applied to codes of over 100,000 lines. A beta version of ADIC (Automatic Differentiation of C) [7] has just been released (see `http://www.mcs.anl.gov/autodiff/adic`).

ADIFOR and ADIC are mainly based on the so-called forward mode of automatic differentiation. Work is underway to extend the ADIFOR/ADIC infrastructure to compute adjoints, and to support parallel language extensions. Prototypes for Fortran are available (ADJIFOR and ADIFOR-MP), and extensions for ADIC are under development. Also, a recently developed module for 2nd order derivatives will shortly be integrated with both ADIFOR and ADIC [8].

A comprehensive overview of currently available automatic differentiation tools in addition to ADIFOR and ADIC can be found at `http://www.mcs.anl.gov/autodiff/adtools`.

4 TWO APPLICATION EXAMPLES

The availability of AD tools that can handle standard computer languages enables accurate derivative-based sensitivity analysis of large computer codes. That is, one need not "simplify" a complicated model (as is often done to make hand-derived derivatives feasible), and one can easily regenerate accurate derivative code whenever the computer model changes. To illustrate, we briefly consider two examples of the successful application of our AD technology for sensitivity analysis. Reports on successful uses of our AD tools in a variety of other application contexts can be found off `http://www.mcs.anl.gov/autodiff`.

4.1 The MM5 Mesoscale Weather Model

MM5 is a 3-D limited area finite-difference weather model capable of both hydrostatic and nonhydrostatic weather simulation and prediction, containing numerous sub-models of various microscale and sub-grid-scale meteorological processes. MM5 has been developed jointly by the Penn State University (PSU) Meteorology Department and the National Center for Atmospheric Research (NCAR) as a community mesoscale model and is continuously being improved by its many users at universities and government laboratories. The MM5 code consists of roughly 40,000 lines of Fortran 77.

In our study, the details of which are presented in [9], we were interested in sensitivities of the forecast generated by MM5 with respect to the initial data. Exploiting the generality of the ADIFOR-generated derivative-enhanced version of MM5, we chose a directional derivative that approximated a so-called Cressman objective analysis scheme, thus investigating the impact of perturbating initial temperature in a limited area of the model at the cost of one directional derivative. These studies revealed an unphysical, low amplitude supersonic precursor wave caused by the acoustic-sound solver employed that would have been invisible even with central divided difference approximations.

4.2 The MaTChM Atmospheric Chemistry Model

The mixed-phase chemistry box model MaTChM is employed at Pacific Northwestern Laboratory to study heterogeneous chemistry and its effect on tropospheric gas-phase chemistry. To determine the impact of the various chemical reaction on the model, an exhaustive sensitivity analysis was performed using ADIFOR. Specifically, the sensitivity of 144 gas, aqueous, and aerosol species with respect to 404 model parameters (245 reaction rate coefficients, 134 mass transport parameters, 21 species initial concentrations, and 4 physical parameters) was computed at every time step.

This study, which is reported in detail in [10, 11], was performed for five different pollutions scenarios, ranging from remote marine to heavily polluted scenarios. The results showed that in some instances previously held beliefs in model sensitivity were not borne out in practice. That is, reactions considered of lesser importance had in fact a pronounced effect on model behavior. In addition, the first round of sensitivity studies helped reveal an error in the original model.

5 CONCLUSIONS

Automatic differentiation enables the accurate computation of derivatives for arbitrary codes. Recently, tools based on this technique have matured to the point where they can be applied to large and complicated simulation codes. Thus, derivative-based sensitivity analysis can now be performed with little human effort and, as illustrated by two examples, it can lead to greatly enhanced insight into a model at hand.

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USING MAYDAY1.2 TO PERFORM UNCERTAINTY AND SENSITIVTY ANALYSIS OF A SYSTEM MODEL

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1 INTRODUCTION

Performing a safety study of a Nuclear High Level Waste Repository is usually planned as an iterative process. Each phase of that process is made up of an Uncertainty and Sensitivity Analysis, which is followed by additional field and laboratory research to obtain more accurate information about the repository. The UA objective is to characterise the uncertainty in the main output variables in the study in order to determine the degree of compliance with the Safety Criteria in the light of the available information. The SA examines which of the input parameters and scenarios are more relevant to those criteria and tries to determine the main knowledge areas to which additicnal research efforts should be devoted. Performing such studies needs the help of a software tool capable of allowing the user to do both types of analysis. MayDay [1], has been designed with that purpose.

MayDay has four parts or models: The 0-Var model, the 1-Var model, the N-Var model and the sampling strategy model. The 0-Var model has been designed to perform the UA. The 1-Var model has been designed to perform SA of one output variable versus one input parameter. The N-Var model has been designed to perform SA when several input parameters are considered as a set, taking into account possible relationships among them. The sampling strategy model allows the user to apply variance reduction techniques.

2 MayDay AS A SOFTWARE TOOL

MayDay has been developed as an interactive tool through which the user selects the variable or variables and the type of analysis he wants to perform. Interactivity is achieved through a graphic user interface, X/Windows under Motif, and a carefully designed core that optimises runtime and CPU resources. MayDay has been developed mainly in C. MayDay has been developed, in its first version, for a 64 bits DEC α/AXP under osf/1 3.0 (DEC-UNIX). The most general environment for MayDay is a local network in which several computers under DOS/Windows, MAC/OS, UNIX or MVS may run the program simultaneously in the DEC α/AXP. The data from probabilistic simulations from any code are written to a binary file specially designed to contain all the important information about the simulations. The data from that file are read with the only non-C subroutine of the code (a FORTRAN77 subroutine) as they are needed in the work session so that execution speed is highly increased.

3 PERFORMING UNCERTAINTY ANALYSIS WITH MayDay

An UA should provide the user the most precise numerical and graphical information about the output variables, conditioned essentially by the sample size. That information will be used to check the compliance of the facility with the safety criteria. So, it is necessary to provide appropriate statistics and graphics to be able to perform that checking. The statistics and graphics implemented in MayDay to perform UA are:

a) General or population statistics (the mean, the Tchebychev, Guttman and normal confidence intervals for the mean, the variance, the geometric mean, the skewness coefficient, the kurtosis,...).
b) Order statistics and their 95% confidence intervals.
c) The histogram.
d) The empirical distribution function, its complementary curve, and their Kolmogorov confidence bands for different confidence levels.

The code lists the values of any input parameter or output variable. Those values may be ordered according to the run number or from the smallest to the largest. All these tools are included in the 0-Var model. In addition to all these

tools, the Kolmogorov, Chi-square and Lilliefors goodness of fit tests [2] are also available in the code. The purpose of including these tests in MayDay is twofold. They may be used to check if input parameters have been properly sampled (the sampled values fit properly their theoretical distributions), and they may be used to check if the output variable samples fit any common distribution (normal, log-normal, exponential,...). The last tool included in the 0-Var model is the Shapiro-Wilk test. this test is used to check the normality of the sample mean in order to decide if the confidence interval under the condition of asymptotic normality of the sample mean may or may not be used.

MayDay includes also a series of tools designed to apply variance reduction techniques. Those techniques are proportional and Neyman's stratified sampling [1], importance sampling using a previous small size sample and ancillary beta distributions (IS) [1], and the Latin Hypercube Sampling (LHS). The following ancillary tools are implemented in the code to apply these techniques. The contribution to the mean plot helps to identify those parts of an input parameter that are related to the highest values of an output variable; if there is any, that plot helps the user in creating strata for the stratified sampling techniques. The stratum subsample size calculation algorithm helps computing the size of subsamples in the different strata. The beta distribution fitting algorithm uses the information provided by the contribution to the mean plot to design ancillary distributions to be sampled in an IS.

4 PERFORMING SENSITIVITY ANALYSIS WITH MayDay

An important problem related to the concept *'Sensitivity Analysis'* is its interpretation. There is no unique interpretation of *sensitivity*. Intuitively, *sensitivity* is related to the concept of the partial derivative of an output variable with respect to an input parameter in a specific point, nevertheless, this interpretation is not suitable to tackle the problem of *sensitivity* in a probabilistic environment. In what follows there is a series of different interpretations of *sensitivity* and the statistics and additional tools implemented in MayDay to cope with those different interpretations of *sensitivity*.

From a probabilistic point of view the most straightforward interpretation of sensitivity is correlation. Correlation is strongly related to linear regressions and measures the strength of the linear behaviour of one variable vs. another one. MayDay includes the Pearson correlation coefficient to measure correlation (1-Var model). The non-parametric version of correlation measures the strength of the monotonic behaviour of one variable vs. another one; the Spearman rank correlation coefficient is implemented with that purpose (1-Var model). An extension of this interpretation of sensitivity is the multiple regression model. In this case an output variable is assumed to be explained through a linear combination of several input parameters. The main difference with simple correlations between one input parameter and an output variable is that possible correlations among the input parameters may dramatically affect sensitivity. The Partial Correlation Coefficients (PCC's) and Standardized Regression Coefficients (SRC's) related to Standardized Regressions are implemented in MayDay to tackle this interpretation of uncertainty (N-Var model). The extension to monotonic models is also considered with the Partial Rank Correlation Coefficients (PRCC's) and the Standardized Rank Regression Coefficients (SRRC's) in the N-Var model. A check on the importance of different input parameters is given by appropriate hypothesis tests in the case of the correlation statistics and by the coefficient of determination (R^2) in the case of the statistics related to the Standardized Regressions.

The techniques mentioned in the previous paragraph fail when they are used to analyze non-linear or non-monotonic models. Several parametric and non-parametric statistics are incorporated to the MayDay 1-Var model to measure sensitivity in these cases, some of them are: The Wilcoxon statistic, the two sample Smirnov statistic, the t statistic, the Kruskal-Wallis and Smirnov k-sample statistics and the Cramer-von Mises statistic. These statistics are suitable to identify relationships between specific regions of an input parameter and an output variable, which is not necessarily associated to a linear or monotonic relationship.

An additional interpretation of *sensitivity* is related to the influence of an input parameter on the final variance of an output variable. In this case an input parameter is important if it may be demonstrated that the uncertainty it is affected by is responsible of a large fraction of the output variable variance. The tool implemented in MayDay N-Var model to detect this type of sensitivity is the Fourier Amplitude Sensitivity Test (FAST) [3]. The last type of sensitivity considered in the SA that MayDay is able to perform is related to the change in the output variable mean and variance that may be induced by changes in the distribution of the input parameters. The latter interpretation is strongly related to the expected benefits of getting new information about the input parameters. Most of the input parameters involved in a Performance Assessment of a Nuclear Waste Repository are affected by knowledge Uncertainty; they are not random in a classical sense, but there is lack of knowledge about them. Additional research could improve the knowledge about them, so that their associated uncertainty could be reduced. In this case further research should be devoted to parameters that could induce a larger decrease in the output uncertainty or in the overall risk associated to the Repository. The estimators of impact in the mean and in the variance [4], are included in the MayDay N-Var model to deal with this interpretation of *sensitivity*.

5 AN APPLICATION TO THE ENRESA PRFORMANCE ASSESSMENT FOR A GENERIC SPANISH REPOSITORY IN GRANITIC ROCK

At the beginning of 1995 ENRESA started a preliminary Performance Assessment for a hypothetical Spanish High Level Waste Repository in a granite generic host rock. The results of this study have recently been published by ENRESA [5]. This Performance Assessment, though preliminary, contains all the elements usually included in a Performance Assessment of any facility of this type. The first step of this work was to explicitly state the Safety Criteria of the Study and the facility design, and to collect all the data about the waste, the host rock and the biosphere. The data corresponding to the last two issues are quite generic. The second step was to develop a series of likely scenarios. The reference scenario was divided in 4 main models and 12 submodels: The basic model (hydrogeologic, thermomechanical and the physical-chemical submodels), the near field model (Inventory, resaturation, canister behaviour, waste release, gas generation and transport submodels), the far field model (colloids and transport submodels), and the biosphere model. Finally, the models were implemented in the code RIP, Miller et al. (1992), consequences were evaluated using a 100 observations random sample. The last step was the uncertainty and sensitivity analysis performed with MayDay.

The results of the uncertainty and sensitivity analysis performed with MayDay were really highlighting, not only for the conclusions about the case study, but also for the general conclusions about uncertainty and sensitivity analysis and their implementation in MayDay. Among the conclusions in the area of uncertainty, the two most important radionuclides were identified, they are ^{129}I at late times (after 7E+4 yr.) and ^{36}Cl at early times (simulations were run until 1E+6 yr.). They were the only real contributors to the dose during all the simulation period. The global maximum dose and maximum doses due to those radionuclides were studied. There was the problem that those distributions are censored in time, since in many runs the dose was still growing, specially in the case of ^{129}I, so that specific estimation procedures are demanded to be implemented in order to avoid that problem. The log-normal shape of the distributions associated to the maximum doses due to different radionuclides that had reached their maximum in all the runs could be checked

Table 1: Statistical data for the maximum dose of the most radionuclides and the total maximum dose. (*)Normal intervals are provided except for these two cases for which Guttmanm intervals are more suitable.

	Lower limit of the 95% confidence interval (normal)	Mean	Upper limit of the 95% confidence interval (normal)	Sample standard deviation	Sample kurtosis
Total	$2.06 \cdot 10^{-6}$	$3.20 \cdot 10^{-6}$	$4.34 \cdot 10^{-6}$	$5.82 \cdot 10^{-7}$	20.9
^{129}I	$2.03 \cdot 10^{-6}$	$3.17 \cdot 10^{-6}$	$4.31 \cdot 10^{-6}$	$5.80 \cdot 10^{-6}$	21.0
^{36}Cl	$1.43 \cdot 10^{-7}$	$2.30 \cdot 10^{-7}$	$3.17 \cdot 10^{-7}$	$4.44 \cdot 10^{-7}$	27.8
^{79}Se	0.0	$9.65 \cdot 10^{-9}$	$3.00 \cdot 10^{-8(*)}$	$7.57 \cdot 10^{-8}$	92.4
^{126}Sn	0.0	$3.12 \cdot 10^{-9}$	$8.90 \cdot 10^{-9(*)}$	$2.15 \cdot 10^{-8}$	47.1

Table 2: Results of several rank standardised regressions for the maximum dose due to ^{129}I

	R^2			
	0.87	0.85	0.82	0.74
Variable	***Partial Rank Correlation Coefficients (PRCC)***			
RMI01	-0.88	-0.87	-0.86	-0.83
R1000	0.70	0.66	0.61	0.55
TRAV1	-0.58	-055	-0.57	---
FOUT1	0.40	0.39	---	---
KDBE1	-0.34	---	---	---

Since the main contributors to risk are those radionuclides shown in table 1, the sensitivity study was essentially focussed on the parameters that more affect the results concerning them, and specially the maximum doses generated by them. The sensitivity study was guided by the standardised regressions in raw values and in ranks. These regressions were done in a sequence beginning with all the parameters that could affect a specific output variable and applying the technique of backward stepwise regression. The results of applying this technique to the maximum dose due to ^{129}I, working on the ranks, are shown in table 3. This table shows that the two main

parameters are the oxidation/alteration rate of the fuel matrix (R1000) and the retardation coefficient of the radionuclide due to matrix diffusion (RMI01), that are the parameters controlling respectively Iodine release from the repository and its movement through the geosphere. When moving from left to right in table 3, the results are updated after removing the regressor with the smallest PRCC (in absolute value) in the last regression.

6 RECENT AND FURTHER DEVELOPMENTS IN MayDay

The work abridged in the previous point of this paper was the first study done with MayDay to analyse data coming from a real large scale performance assessment, and it was a good check for its real power and weaknesses. As a result of the lessons learned in that study, the following new tools and modifications of existing tools were decided to be implemented in the code :

a) A tester of the quality of the sample that checks if the sample fits the conditions under which it was supposed that was going to be produced. This tester checks the fit of the input parameter samples to their theoretical distributions and the correlation between different pairs of input parameter samples. This statistic shows if the number of poor fits or wrongly induced correlations (whichever its cause could be) exceeds the limit number expected in sampling theory.
b) Simple transformations and combinations of the variables in the binary file are allowed, like crossed products, pure squares, logarithms and the inverse, among others. All these transformations and combinations are done interactively, avoiding manipulation of files outside the program.
c) Inclusion of new distributions in the code : Exponential, Weibull and log-triangular.
d) Modifications of different statistics to improve their interactivity.

In addition to the aforementioned developments, which have recently been implemented in the code, the following tasks are planned for the year 1998:

a) To provide the code specific graphical and statistical tools to show the evolution of risk and its uncertainty in time.
b) To provide the code tools to edit interactively the binary file, modifying or adding data as needed by the user
c) Reprogramming the whole code in double precision.

7 ACKNOWLEDGEMENTS

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COMPARISON OF SOME METHODS FOR SENSITIVITY ANALYSIS OF DISCRETE EVENT SYSTEMS SIMULATION MODELS

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1 INTRODUCTION

Discrete event systems (DES) Simulation models are not only limited by the construction, besides they should respond to the exigency and hope in the application for which they are planed. Generally, a simulation model is constructed due to the difficulty in finding a mathematical model to represent the real system (communication networks, computer systems, production lines, traffic systems). Simulation models permit to study some performance measures, see e.g. [1, 2].

On the other hand, there are so complicated DES that they make practically impossible to obtain the analytical form of the performance measure called $j(\Theta)$, where Θ is a vector of system's parameters.

Examples of such performance measures are averages of some system variables, such as, average waiting time in system, average number of entities per period at system, time-project average in PERT network.

It could be of interest to the system manager or to the system analyst, to find out the influence of some of the system parameters on its performance.

This situation induces to think about the following questions:

How can we estimate the derivatives of mean values respect to various parameters?

Which method would be advantageous to use in our simulation model for estimating such derivatives?

The last question emerges because there are various methods for estimating such derivatives. They were developed in the last 20 years, some of them are perturbation analysis family, likelihood ratios method, score function method and finite difference method; see e.g., [3, 4, 5, 6, 7].

In this paper, we present a new systematic way to select the method for estimating derivatives of the performance measures. This method is based on a new DES taxonomy and on the characteristic of each sensitivity method.

The paper as a whole is organized as follows: In the next section we present some definitions. Subsequently, we show the methodology employed, the selection sensitivity method (main result) through algorithm. An example is presented to explain the selection sensitivity method. Finally we give concluding remarks.

2 DEFINITIONS

In this section, we present a brief explanation of the general characteristic of each studied sensitivity method.

Perturbation Analysis Method Family

The perturbation analysis (PA) method family calculates the sensitivity of performance measure (PM) of discrete events dynamic systems (DEDS) with respect to system parameters by analyzing its sample path, see e.g. [3, 8, 9, 10, 11]. This method family is based on the generation of the perturbed path (sample path for the case in which the parameter (e.g. θ) is increased (to $\theta+\Delta\theta$)) simultaneously with the nominal path (sample path for the case with parameter in nominal value).

The temporal infinitesimal perturbation analysis (TIPA), so named by the authors to differentiate it from the structural infinitesimal performance analysis (SIPA) method, see e.g. [4]. TIPA estimates the sensitivity of PM with respect to parameters that determine timing system quantities, also called timing parameters, see e.g. [3, 8, 9, 12]. On other words, those parameter quantities that are defined by random clocks associated with the possible events on a system state, in the generalized semi-Markov processes (GSMP) sense, see e.g. [3, 12, 13, 15].

The SIPA computes the sensitivity of PM with respect to structural parameters, that is to say, those parameters that can modify the stochastic state transition probability, in the GSMP sense, see e.g. [4].

The smoothed perturbation analysis (SPA) method is a variety of TIPA. This method is used to estimate sensitivity of PM with respect to parameters, when there are the effect of possible discontinuities in the sample performance path caused by perturbation of parameters, because the deterministic similarity between the nominal path and the perturbation path is violated, see e.g. [3, 11].

Discontinuous perturbation analysis (DPA) method was developed to estimate sensitivity of PM with respect to parameters, in the case that the sample PM has discontinuity especially due to threshold type of parameters or structure parameter, see e.g. [11].

Score Function Method

A previous analysis of sample path is not required by this method. The score function (SF) method is based, from a methodology approach, on the sampling of the PM and the so-called score function. This method satisfactorily estimates sensitivity of PM on discrete event static systems (DESS), nevertheless, the method can be used on DEDS, see e.g. [5, 15].

Likelihood Ratios Method

A similar approach to SF by the likelihood ratios (LR) method is presented, nevertheless, LR method is used to estimate sensitivity of PM with respect to Poisson random variable associated parameters. On the other hand, LR can be used in the study of constant or variable Poisson parameters, see e.g. [6].

Finite-Difference Method

Finite-Difference (FD) method is based on classical derivatives definition. Diverse approach have been shown in many references, e.g. [7, 16].

3 METHODOLOGY

The methodology employed on the selection of sensitivity method on DES was: in the first place, to study the extent and limitation of each sensitivity method, e.g. [17]; second, to develop a taxonomy hierarchy to be used on SED simulation models, from sensitivity analysis approach and considering the taxonomy principles, see e.g. [18]. With this step we get the following hierarchy kind:

Evolution: The DES can be classified in: dynamic or static.

Parameter: The parameters are classified in: timing or structural.

Poisson: Also the parameters can be: Poisson or non Poisson.

Variable: The parameter can influence the sample PM: continuous or discontinuous.

Constructive: The path can be constructive or not.

Similarity: The path can be of deterministic similarity or not.

4 SELECTION SENSITIVITY METHOD

This method is shown through the following algorithm, e.g. [17].

Let $j(\Theta)$ be the PM of DES of which we wish to estimate the sensitivity with respect to its parameters.

For each parameter of the DES,

1) Test: If the SED is a dynamic model then go to 4, else go to 2
2) Test: If the SED model satisfying condition to use SF method then go to 3, else go to 21
3) Output: To employ SF method.
4) Test: If the parameter is structural then go to 5, else go to 7
5) Test: If the SED model satisfy the condition to use the SIPA method then go to 6, else go to 21
6) Output: To employ SIPA method.
7) Test: If the parameter is Poisson then go to 8, else go to 12
8) Test: If the parameter is variable then go to 9, else go to 10
9) Test: If the SED model satisfy the condition to use the LR method then go to 11, else go to 21
10) Test: If the SED model satisfy the condition to use the LR method then go to 11, else go to 12
11) Output: To employ LR method.
12) Test: If the behavior of PM is discontinuous with respect to the parameter then go to 13, else go to 15
13) Test: If the SED model satisfy the condition to use the DPA method then go to 14, else go to 15
14) Output: To employ DPA method.
15) Test: If the path of PM is constructive then go to 16, else go to 21
16) Test: If the path has deterministic similarity go to 19, else go to 17
17) Test: If the SED model satisfy the condition to use the SPA method then go to 18, else go to 21
18) Output: To employ SPA method.
19) Test: If the SED model satisfy the condition to use the TIPA method then go to 20, else go to 21
20) Output: To employ TIPA method.
21) Output: To employ FD method.

5 EXAMPLE

The system considered here consists of M/M/1/∞ queue (Q) and customer served in a First-In, First-Out manner. The customer goes back with probability (1-p) immediately after it leaves the server (S) or goes out of system with probability p, see fig. 1. The interarrival and service times are exponentially distributed with interarrival and service rate λa and λs, respectively. The PM considered here is the average time spent by the customers in the system, denoted as $T_S(\lambda a,\lambda s,p)$. The decision p parameter is the probability that a customer goes out of the system.

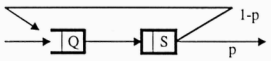

Figure 1. M/M/1/∞ queue with feedback

We wish to estimate the sensitivity of $T_S(\lambda a,\lambda s,p)$ with respect to p parameters and as an end product of the selection sensitivity method algorithm, the sensitivity of the PM can be estimated through SIPA method, see e.g. [17].

6 CONCLUSIONS

This method based on DES taxonomy and the illustrated algorithm, gives to the system analyst a guide or methodology to estimate the sensitivity of the performance measure of discrete events systems.

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AN INVERSE APPROACH TO ANALYSE SOIL MOISTURE FROM OBSERVATIONS OF ATMOSPHERIC TEMPERATURE AND HUMIDITY

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1 INTRODUCTION

Soil moisture transport across the air-soil interface and in the upper layers of the earth's surface is one of the important links in the energy and water cycle of the earth, connecting hydrology, meteorology, and climate research. In atmospheric modeling, specification of soil moisture determines to a large extent the relative magnitudes of sensible and latent heat fluxes. Its incorrect specification may downgrade the atmospheric weather forecast over longer times. Unfortunately soil moisture is not observed on a routine basis.

Mahfouf [1] proposed a method to retrieve information on soil moisture from atmospheric observations through inverse methods. In this study we apply a variational data assimilation approach which fits the model trajectory over some time interval to data using the model equations as a strong constraint. Our model predicts the evolution of soil variables and atmospheric tendencies originating from soil physics and turbulent transports in the atmospheric boundary layer. Horizontal advection is neglected. The system is driven by specification of atmospheric state variables at its upper boundary and radiative fluxes at the surface.

Though it is not necessarily needed for our low-dimensional variational problem, we provided the adjoint code of our model since it is a valuable tool for all sensitivity studies related to the assimilation problem [2]. The code has been produced by using the automatic differentiation tool IMAS [3, 4].

2 RETRIEVAL OF SOIL MOISTURE

The goal is to find a suitable initial soil moisture value η so that the model predicted $2m-$temperatures $T(\eta, t_{obs})$ and relative humidities $RH(\eta, t_{obs})$ at observational time t_{obs} come close to the observations T_{obs}, RH_{obs}. Technically the minimum of the following cost function J has to be found:

$$J(\eta) = \frac{1}{2} \sum_{obs} \frac{(T(\eta, t_{obs}) - T_{obs})^2}{{\sigma_T}^2} + \frac{(RH(\eta, t_{obs}) - RH_{obs})^2}{{\sigma_{RH}}^2} \; .$$

We consider 23 observations at a meteorological station near Braunschweig (Northern Germany) between 0 and 24 UTC on March 5, 1994. The observational error standard deviations are estimated to be $\sigma_T = 1\mathrm{K}$ and $\sigma_{RH} = 10\%$.

Operationally predicted temperatures for the same location where systematically lower than the observed ones, while relative humidities where too high with virtually no diurnal cycle (solid lines in the two panels of Fig. 1). After initial soil moisture optimization, re-running the model reveals a forcast which fits much better the observations. The dotted line shows the effect of trying to adjust radiative forcing instead of soil moisture. Although predicted temperatures come close to the observations, this is not true for relative humidity.

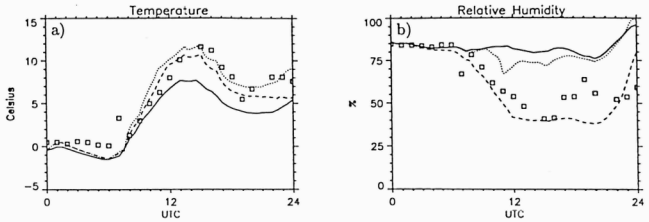

Figure 1: Atmospheric Temperatures (a) and Relative Humidities (b), both at 2m - Height: Operational forecasts (solid), Recalculations with Retrieved Initial Soil Moisture (dashed), Recalculations with Adapted Solar Radiation (dotted). Symbols: Observations.

3 SENSITIVITY STUDIES

The tangent-linear model provides information on the effects of infinitesimal perturbations in initial conditions. Fig. 2a) shows the results of differentiating $2m$ dew point temperatures (representing absolute atmosheric humidity) at each time step of the calculated model trajectory over 24 hours with respect to lower soil layer temperature T_2 at initial time 0 UTC. The temporal evolution of the partial derivatives has a rather complex structure. Before sun rise, the regular increase in sensitivity reflects the time scale of thermal diffusion in the upper soil. After sun rise, the abrupt changes in the sensitivities can be attributed to the successive coupling or decoupling of atmospheric model layers by turbulent diffusion, depending on the actual strength of radiative heating.

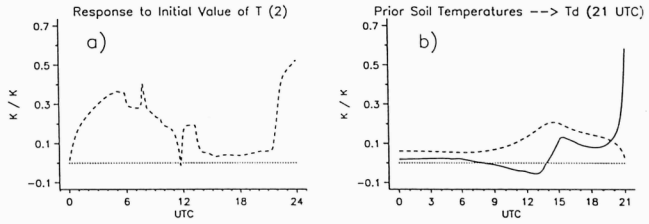

Figure 2: a) Partial Derivatives of 2m - Dew Point Temperatures (dashed), with respect to Lower Soil Temperature T_2 and b) Partial Derivatives of Dew Point Temperature at 21 UTC with respect to Surface Temperature T_1 (solid) and Soil Temperature T_2 (dashed) at all prior times.

According to Fig. 2a, the response of atmospheric dew point temperature (absolute humidity) at 21 UTC to a perturbation in soil temperature inserted at initial time 0 UTC is relatively weak. This leads to the more general question of how the same observation at 21 UTC would be influenced by a soil temperature perturbation inserted at any other time between 0 UTC and 21 UTC. The answer to this question (Fig. 2b) can be gained efficiently from running an adjoint model.

T_1 denotes the surface temperature being in direct contact with the atmosphere and triggering the soil-atmosphere exchange processes as well as the turbulent transports in the atmospheric boundary layer. According to Fig. 2b, the impact of a T_1-disturbance on dew point temperature at 21 UTC

(solid line) may be positive or negative depending on the time of its insertion. The essential change in sensitivity occurs around 14 UTC when the atmospheric turbulent boundary layer has reached its maximum height.

The sensitivities of dew point temperature with respect to prior values of deeper soil temperature T_2 can be understood by realizing that 1.) T_2 represents a layer with a certain thermal inertia and 2.) the influence of T_2 on the atmosphere is an indirect one channeled through prior interaction with T_1. These two aspects may be combined in assuming that the sensitivity of dew point temperature T_d with respect to T_2 originates from that with respect to T_1 by low pass filtering according to the following differential equation,

$$\frac{dg_2}{d\tau} = -kg_2 + bg_1 \;\; ; \;\; g_2(0) = 0, \;\; \Longrightarrow \;\; g_2(\tau) = b\int_0^\tau g_1(\tau')e^{k(\tau'-\tau)}d\tau' \;\; ,$$

where $g_i = \frac{\partial T_d}{\partial T_i}$. The delay time τ is defined as the difference between actual time t and observational time ($\tau = t_{21} - t$ with $t_{21} = 21\ UTC$). An excellent fit to g_2 (i.e. the dashed line in Fig. 2b) is obtained by choosing $k = (8.75\ hrs)^{-1}$ and $b = (2.75\ hrs)^{-1}$.

From our analysis we conclude, that the weak influence of soil temperature T_2 at 0 UTC on the atmospheric dew point in the evening originates from two different sources. First, the marked influence of T_2 via T_1 on the atmosphere has a tendency to compensate on average due to different signs in the course of the day. Second, the time an energy signal persists in the soil layer represented by T_2 is less than the assimilation interval of 21 hours.

4 IMPACT OF OBSERVATION TYPE

When retrieving soil moisture from an optimization of atmospheric forecasts, we implicitly assume that soil moisture alone is responsible for possible failures to forecast the observed atmospheric variables. A key condition for an operational implementation of the method is its stability against other, uncertain model components. Model errors (outside the scope of modeling surface fluxes as functions of soil moisture) should have little effect upon analyzed soil moisture values.

A particularly important error source is the calculation of radiative forcing which crucially depends on specification of cloud cover, for instance. We will demonstrate that the control variables soil moisture and radiative forcing exploit different pieces of information, so that the impact of soil moisture on the atmospheric boundary layer remains identifiable even in the presence of significant radiation errors.

From Figs. 1 we saw that atmospheric relative humidity is much less sensitive with respect to misspecified radiative forcing than is atmospheric temperature. The response of atmospheric temperature with respect to stronger radiative forcing is very much the same as its response to lower soil moisture. That means that if we assign to radiative forcing the status of a control variable (instead of supplying its value from outside), the task of optimizing soil moisture and radiative forcing at the same time will become an ill-posed problem. However, including atmospheric relative humidity as an additional source of information remedies the ill-posedness and makes retrieved soil moistures stable with respect to erroneous radiative forcing.

To illustrate this behaviour, Fig. 3 depicts the results of soil moisture analysis over Central Europe on the 5^{th} of March 1994. Assimilation has been performed for each grid cell ($14 \times 14 \mathrm{km}^2$) independently (no horizontal advection). Each locally prescribed radiative flux has been multiplied by some individual correction factor which then has been retrieved together with soil humidity by minimizing the distance between data and the model trajectory.

The left column of panels in Fig. 3 shows the retrieved soil moistures when using atmospheric temperature plus relative humidity as data input (upper panel) or temperature data alone (lower panel). The right column of panels depicts the respective optimum radiation correction factors. It can easily be recognized that the fields in the first row of Fig. 3 are much smoother than the fields in the second row. When using temperature information alone (lower panels), responsibility for dicrepancies between data and model simulation is assigned in an erratic way to one of the two control variables. If, however, information on atmospheric relative humidity is included, the analysis yields a considerably smoother distribution of soil moisture and radiative forcing as well. This indicates that relative humidity, not temperature is the main observational parameter which provides information on soil humidity if radiative forcing is uncertain.

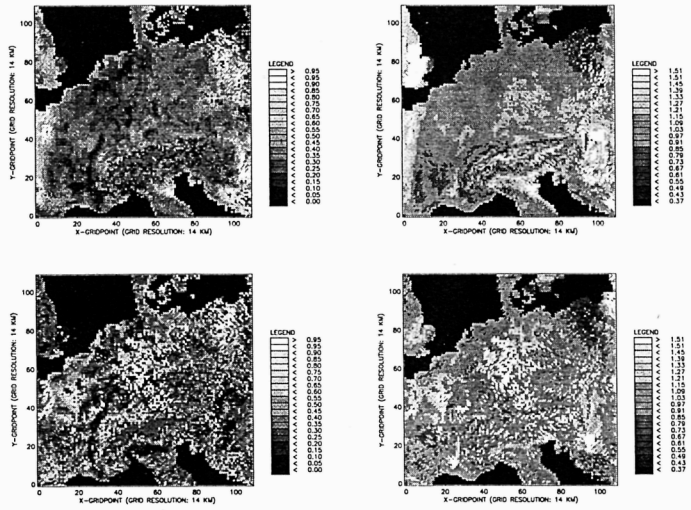

Figure 3: Upper Panels: Retrieved Soil Moisture Normalized with its Saturation Value (left) and Radiation Correction Factor (right) when using Observations of Atmospheric Temperature and Relative Humidity as well. Lower Panels: Same as Upper Panels but Excluding Information on Relative Humidity.

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THE USE OF GRAPH THEORY IN THE SENSITIVITY ANALYSIS OF THE MODEL OUTPUT. A NEW SCREENING METHOD.

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Sensitivity analysis screening methods aim to isolate the most important factors from amongst a large number that may affect a particular response [1,2,4,5].

In dealing with models which are computationally expensive to evaluate and which have a large number of input parameters, it is very important to adopt methods which are "economic", i.e. which require a relatively small number of model evaluations. These computationally efficient sensitivity analysis techniques include the 'one-factor-at-a-time', or OAT, screening designs [3,4]. The OAT techniques assess the impact on the output of changing one parameter value at a time, and are based on the assumption of absence of effects (on the model output) due to the interactions among input factors. In other words, the input variables are assumed to act additively, i.e. the effects due to two parameters, say x_i and x_j, are all amenable to the linear combination of the effects of x_i and x_j.

This assumption, although undesirable, is needed in order to simplify the problem and keep low the computational cost of the experiment. Methods rejecting such an assumption, and computing higher order effects, (i.e. the class of the Factorial Designs), are computationally expensive, and their computational cost increases with the number of levels across which the model input variables are varied.

The OAT screening method proposed by Morris [4], requires an order of k, $O(k)$, model evaluations where k is the number of model input factors, and provides sensitivity estimates of the 'total' effect (i.e. the sum of first and higher order effects due to a single parameter), and an 'overall' sensitivity measure of curvature and interactions between factors. The main advantage of the Morris method is then its economy in running time. As a drawback, the 'overall' sensitivity measure given by Morris does not distinguish non linear from interaction effects, and does not provide distinct sensitivity measures for each possible two-factor, three-factor or higher interactions.

This paper shows how the Morris method can be extended to develop information on two-factor interactions, whilst still retaining its computational efficiency.

Assume that the model output $y = y(\mathbf{x})$ is a scalar function of the vector of input factors $\mathbf{x} = (x_1, x_2, .., x_k)$, whose components x_i can assume integer values or levels in the set {0,..., p-1}.

The Morris technique is based on the definition of an *elementary effect* attributable to an input factor. For a given value of $\mathbf{x}$, the *elementary effect* for the ith input factor is defined as

$$d_i(\mathbf{x}) = [y(x_1, \ldots, x_{i-1}, x_i + \Delta, \ldots x_k) - y(\mathbf{x})] / \Delta,$$

where Δ is a predetermined integer selected in {1,2,..., p-1} and $\mathbf{x}$ is any selected vector in Ω such that the transformed $(\mathbf{x} + \Delta)$ is still in Ω.

The purpose of the experimental plan is collecting random samples from each distribution F_i of elementary effects associated with each input factors. Analysis of those distributions will assess the relative importance of the input factors: a large measure of the distribution mean value, μ, indicates an input factor with an high "overall" influence on the output, while a high value of standard deviation, σ, indicates an input factor that is involved in interactions with other factors or whose effect is non-linear.

In the new method, for a given value of the input vector x, selected in the parameter space Ω, the *elementary effect* EE_{ij} $(1 \le i < j \le k)$, attributable to the pair of *i*th and *j*th input factors, is defined as

$$EE_{ij}(\mathbf{x}) = [y(\mathbf{x} + \mathbf{e}_i\Delta_i + \mathbf{e}_j\Delta_j) - y(\mathbf{x})] / \Delta_i\Delta_j,$$

where $\Delta=(\Delta_1,\ldots,\Delta_k)$ is a predetermined vector such that the transformed $(\mathbf{x} + \mathbf{e}_i\Delta_i + \mathbf{e}_j\Delta_j)$ is still in Ω. The distribution of EE_{ij}'s is denoted by F_{ij}.

The quantities EE_{ij} can be used in order to provide a measure of the effect on the output due to the interaction between the *i*th and the *j*th input factors. In facts, such an effect can be measured by computing the partial derivative of the output function *y*, with respect to its input variables x_i and x_j. An approximation for this derivative is given by

$$\frac{\partial^2 y}{\partial x_i \partial x_j} \cong EE_{ij} - \frac{1}{\Delta_i} EE_i - \frac{1}{\Delta_j} EE_j,$$

where EE_i and EE_j are the elementary effects defined above.

It follows that, in the point $\mathbf{x} = (x_1, x_2, .., x_k)$ of the parameter space, the two-factor interaction effect due to x_i and x_j can be estimated by the quantity TFE_{ij} defined as

$$TFE_{ij} = \left| EE_{ij} - \frac{1}{\Delta_i} EE_i - \frac{1}{\Delta_j} EE_j \right|.$$

Denote by T_{ij}, the distribution of the TFE_{ij}'s, obtained by varying the point x in the parameter space. The estimated mean $\lambda(i, j)$ of the distribution T_{ij}, can be considered as global sensitivity measures of the two-factor interactions: a high value of $\lambda(i, j)$ indicates a pair of input factors largely affecting the output through their mutual interaction; a value of $\lambda(i, j)$ which is close to zero indicates that the *i*th and *j*th input factors are acting independently on the output.

Estimates of the means of the T_{ij} distributions are obtained by using an efficient sampling strategy in the parameter space which is based on notions of graph theory and, in particular, on the solution of the 'handcuffed

prisoner problem'. The computational cost of the experiment is of the order of k^2, and it does depend on the number of 'levels' selected for each parameter.

Results obtained on analytical test functions -including the one used by Morris [4]- confirm that the three sensitivity measures λ, μ, and σ, provide high level of information about the relative importance of the input factors, and the nature of their effects on the output.

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WINDING STAIRS AS A TOOL TO GENERATE SAMPLES FOR SENSITIVITY ANALYSIS

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1 INTRODUCTION

This paper describes a sampling scheme used to perform sensitivity analysis (SA) of model output. In general, SA is conducted by the following steps: (i) defining a model which approximates economic, engineering, environmental, physical or social phenomenon of various levels of complexity, and its input parameters and output variable(s); (ii) assigning probability distributions to the input parameters; (iii) generating input values via an appropriate random sampling method and evaluating the output; and (iv) assessing the influence or relative importance of each input parameter on the output variable. This paper is devoted to steps (iii) and (iv).

Here, we assume a model output Y is depended on k input parameters, say $x_1, x_2, \cdots, x_k$, namely

$$y = f(x_1, x_2, \cdots, x_k).$$

Difficulty can arise from within a modelling process when the model parameters are not constant, but vary in some manner about nominal values. We model out certainty about the values of the inputs by treating them as random variables. Hence, when modelling real world phenomena with numerical experiments (a mathematical model) one is often faced with the problem of what values to use for the inputs. In SA, several values of $\mathbf{X}$, say $\mathbf{X_1}, \mathbf{X_2}, \cdots, \mathbf{X_n}$ are generated as successive sets of inputs in order to obtain the desired information concerning Y.

For some complex models, the computational cost can be expensive in terms of number of model evaluations. The sample size, n, should be small to minimise the computational cost, hence the values of the input variables should be selected with great care. Several techniques to generate sample input points, such as Crude Monte Carlo, Latin hypercube, Sobol' LP_τ, have been applied and compared ([1] and references therein).

The next section describes a method of selecting (sampling) input parameter. In that section methods for assessing the influence or relative importance of each input parameter on the output variable are also given. An example which illustrates the method is presented in Section 3; also in that section a brief discussion is given.

2 THE WINDING STAIRS SAMPLING METHOD

In ordinary Monte Carlo (MC) sampling a new realisation of the model output y is obtained by drawing new values for the inputs according to their joint probability distribution, and calculating y after *all* new drawings. Such a sample contains no information about the role of the individual input parameters.

The winding stairs method [2] consists of calculating y after each drawing of new value of an individual source, x_i for $i = 1, 2, \cdots, k$. In this method, we assume that the input parameters, X_i's, are stochastically independently distributed, that is $p(\mathbf{x}) = \prod_{i=1}^{k} p_i(x_i)$ where p_i is the probability distribution of parameter X_i. This assumption allows us to draw a value at random from each input parameter space using a pseudo-random number generator. A sequence of sample points is generated as follows:

> we generate a value from each of the input parameter space to obtain a sample point in the k dimensional parameter space, e.g. $\{x_{11}, x_{21}, x_{31}, \cdots, x_{k1}\}$. (Note that the first suffix denotes

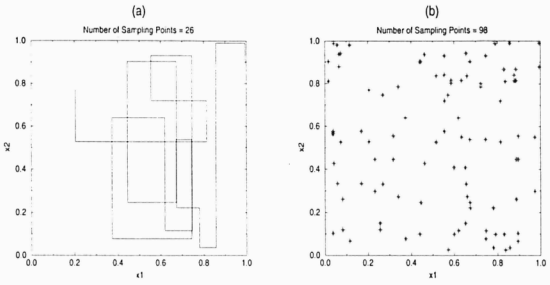

Figure 1: Plots of sample points generated by the Winding Stairs method in the two-dimensional case.

parameter number and the second suffix denotes sample number.); we then sample a value from the sample space of the second parameter to obtain a second sample point, namely $\{x_{11}, \mathbf{x_{22}}, x_{31}, \cdots, x_{k1}\}$. Similarly, a third sample point is obtained by sampling a value from sample space of the third parameter giving $\{x_{11}, x_{22}, \mathbf{x_{32}}, \cdots, x_{k1}\}$, and so on. Hence, the kth sample point is $\{x_{11}, x_{22}, x_{32}, \cdots, \mathbf{x_{k2}}\}$ and the next sampling point is obtained by changing the value of the first parameter giving, $\{\mathbf{x_{12}}, x_{22}, x_{32}, \cdots, x_{k2}\}$. We repeat these steps until we obtain the desired number of sample points.

This means that new input values are sampled in a fixed *cyclic* order. The output is evaluated after each sample input point is generated, yielding a sequence of output y_l, for $l = 1, 2, \cdots, N$, where N is the total number of model evaluations. If we arrange the sequence of N output into k columns and r rows where r $(= N/k)$ is the number of turns to repeat the cyclic order, then the entries within each columns are independent of each other. The consecutive points within each row are not independent in the sense that the points differ in a single input value. In practice (see below), we generate $k \times (r+1)$ input points. Figure 1(a) shows the path of a sequence of 26 sample points, generated by the WS Sampling scheme in a 2 parameter case; a plot of 98 (with k=2 & r = 48) WS sample points is given in Figure 1(b).

The ultimate goal in performing SA is to investigate the relative importance of each input parameter. This could be done by measuring the main effect and/or total effect of each individual input parameter on the model output. The main effects can be measured by the so-called partial variance or correlation ratios (for discussion of these two measures see [3]), or the Top Marginal Variance (TMV) [2], which is defined to be the expected variance reduction due to fixing of parameter x_i while the remaining $\mathbf{x}_{\sim i}$ vary. Here $\mathbf{x}_{\sim i}$ denotes a vector of input values $\mathbf{x}$ excluding the input value for parameter x_i.

Jansen *et al* [2] proposed to measure the main effect of parameter x_i, denoted by D_i here, by the following

$$D_i = D - \frac{1}{2} E\left[f(X_i, \mathbf{X}_{\sim i}) - f(X_i, \mathbf{X}'_{\sim i})\right]^2, \tag{1}$$

where D is the output variance. Since the output within each column are independent of each other, D can be estimated by pooling all the k sample variances of the r independent output. Hence, the WS sample estimate of D is given by

$$\hat{D}^{WS} = \frac{1}{k(r-1)} \sum_{i=1}^{k} \sum_{m=1}^{r} f^2(x_{im}) - \frac{1}{r} \left[\sum_{m=1}^{r} f(x_{im})\right]^2. \tag{2}$$

The right hand side of Equation (1) can be estimated by using the r by k WS output matrix described above, namely

$$\hat{D}_i^{WS} = \hat{D}^{WS} - \frac{1}{2r} \sum_{l=i}^{r} \left[y_{k(l-1)+i} - y_{kl+i-1}\right]^2.$$

For example, with $k = 6$ and $r = 4$ to compute $\hat{D}_1^{WS}$ we calculate the squared difference between the first and the 4th column of the first 4 rows of the output matrix. However, for the second parameter x_2, the squared differences are computed using the values in column 1 and column 2, i.e. $\{y_7, y_{13}, y_{19}, y_{25}\}$ and $\{y_2, y_8, y_{14}, y_{20}\}$ respectively.

Jansen [4] showed that

$$D - \frac{1}{2}E\left[f(X_i, \mathbf{X}_{\sim i}) - f(X_i, \mathbf{X}'_{\sim i})\right]^2 = Cov\left[f(X_i, \mathbf{X}_{\sim i}), f(X_i, \mathbf{X}'_{\sim i})\right]. \tag{3}$$

The estimate of the right hand side of Equation (3) can be obtained by performing MC integral, namely

$$\widehat{Cov}\left[f(X_i, \mathbf{X}_{\sim i}), f(X_i, \mathbf{X}'_{\sim i})\right] = \frac{1}{n}\sum_{j=1}^{n} f(x_{ij}, \mathbf{x}_{\sim ij}) f(x_{ij}, \mathbf{x}'_{\sim ij}) - \hat{f}_0^2, \tag{4}$$

where n is the sample size to generate tthe data matrix (see [5]) and $\hat{f}_0 = \frac{1}{n}\sum_{m=1}^{n} f(\mathbf{x}_m)$ is a sample estimate of the mean model output. The right hand side of Equation (4) provides an estimate of the partial variance, D_i, proposed by [6] in that the first order sensitivity index for parameter x_i, denoted by S_i, was defined. It is estimated by $\hat{D}_i/\hat{D}$, where D is estimated by the sample variance, namely $\frac{1}{n}\sum_{m=1}^{n} f^2(\mathbf{x}_m) - \hat{f}_0^2$. Hence, the WS sample estimate of the S_i is given by

$$\hat{S}_i^{WS} = 1 - \hat{D}_{\sim i}^{WS}/\hat{D}^{WS}.$$

Similarly, it can be shown (see [7]) that

$$D - \frac{1}{2}E\left[f(X_i, \mathbf{X}_{\sim i}) - f(X'_i, \mathbf{X}_{\sim i})\right]^2 = Cov\left[f(X_i, \mathbf{X}_{\sim i}), f(X'_i, \mathbf{X}_{\sim i})\right]. \tag{5}$$

Again, the right hand side of Equation (5) can be estimated by

$$\hat{D}_{\sim i} = \frac{1}{n}\sum_{m=1}^{n} f(x_{im}, \mathbf{x}_{\sim im}) f(x'_{im}, \mathbf{x}_{\sim im}) - \hat{f}_0^2 \tag{6}$$

In [5], Equation (6) is used to compute the so-called Total Sensitivity Index (TSI), which measures the total influence of an individual parameter on the model output variation and is defined as the sum of all the sensitivity indices (including all the interaction effects) involving the parameter of interest (for further explanation see [3]). The TSI of parameter x_i, denoted by TS_i, is given by $TS_i = 1 - S_{\sim i}$, where $S_{\sim i}$ is the sum of all the indices which do not include parameter x_i and is computed by $\hat{D}_{\sim i}/\hat{D}$. ¿From Equation (5), the TSI can be estimated by subtracting the mean of half of the squared differences between $f(X_i, \mathbf{X}_{\sim i})$ and $f(X'_i, \mathbf{X}_{\sim i})$ from the total output variance, D. Hence, the WS sample estimates of TSI for parameter x_i is given by

$$\widehat{TS}_i^{WS} = \begin{cases} \frac{1}{2r}\sum_{l=1}^{r}\left[y_{lk} - y_{lk+1}\right]^2/\hat{D}^{WS} & \text{if } i = 1 \\ \frac{1}{2r}\sum_{l=1}^{r}\left[y_{k(l-1)+i-1} - y_{k(l-1)+i}\right]^2/\hat{D}^{WS} & \text{if } i \neq 1 \end{cases} \tag{7}$$

where $\hat{D}^{WS}$ is given in Equation (2).

The efficiency of the winding stairs method lies mainly in the multiple use of model evaluations. In computing either the first order or the total sensitivity indices for all the parameters, in general, one model evaluation is used twice.

3 AN ILLUSTRATION AND DISCUSSION

In this section we describe a small simulation study to illustrate the WS sampling method to estimate the first order and total sensitivity indices. In this study we use the g-function described in [7] and the number of input parameters used is eight; the values of a_i are chosen to be $\{0, 1, 4.5, 9, 99, 99, 99, 99\}$. The experiment is performed repeatedly so that the accuracy and precision of the sampling method can be assessed. Results of an extensive simulation study to compare the WS sampling technique with the Sobol' method are described and discussed in [7].

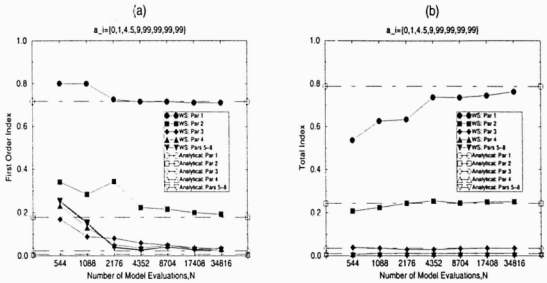

Figure 2: An illustration: WS estimates of the First Order and Total Sensitivity Indices

Figure 2(a) shows a plot of the WS estimates of the first order sensitivity indices against numbers of model evaluations for all eight parameters. Preliminary results suggested that WS method provides reasonable estimates of first order sensitivity indices for important parameters at low sample size; while the estimates for unimportant parameters are not so accurate at low sample size but converge to the analytical values as the number of model evaluation increases.

Figure 2(b) shows a plot of the WS estimates of the total sensitivity indices against numbers of model evaluations for all eight parameters. With a very low number of model evaluations, the WS method appears to give better estimates of TSI for unimportant parameters than for important parameters.

The main advantage of the winding stairs sampling method is the multiple use of model evaluations, in that the first order and total sensitivity indices of each parameter can be computed using a single set of model evaluations. In computing both the first and total indices, with the same sample size, WS uses $k \times n$ model evaluations, comparing with the Sobol', $n(2k+1)$; a saving of more than half of the model evaluations.

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MODEL SELECTION BY PARAMETRIC BOOTSTRAPPING: A POWERFUL ALTERNATIVE TO BAYES

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1 INTRODUCTION

The variability of simulation output can be attributed broadly to two causes: that due to uncertainty in the values of input parameters used in the model of the system under study (*parameter uncertainty*) and that due to random variation introduced in the simulation to represent chance behaviour of the system itself (*simulation uncertainty*). Sensitivity analysis clearly needs to take both into account in assessing simulation variability. Cheng and Holland [1] have shown that to a first approximation the two types of uncertainty can be analysed separately. They also point out that parameter uncertainty covers not simply parameter uncertainty, but can be extended to cover the case of *model uncertainty*, where there is uncertainty as to the correct form of the model being used.

We discuss this issue of model uncertainty, and consider how it can be handled as a particular case of parameter uncertainty. We review two approaches that have been proposed in the literature.

One is the *non-nested model* approach which to date has relied mainly on classical methods of statistical inference (See, for example [2, 3]). However such classical methods run into difficulty, as the problem is known to be non-regular, so that standard methods based on asymptotic normality theory do not usually apply. The fitting of *finite mixture models* which is essentially the approach we shall adopt, can be regarded as a variant of this approach; this also non-regular in nature and a discussion is given in [4] and in [5].

The other is the *Bayesian* approach. This has been the subject of recent active study (see for example [6, 7]), mainly because of the development of practical numerical methods of generating posterior distributions through use of Markov Chain Monte Carlo (MCMC) methods. Such Bayesian methods require the choice of appropriate prior distributions. In the context model uncertainty, the form of the posterior distribution, and resulting inference, turn out to be especially sensitive to the choice of prior, making this choice a delicate one. Moreover it is not entirely clear how the Bayesian approach handles the non-regularity, which is still inherent in the problem.

We propose in this paper a classical, rather than Bayesian, formulation but where the difficulty involving non-regularity is addressed and accounted for. The method uses a parametric bootstrap, which vies with MCMC in providing a powerful numerical approach especially for complicated and difficult problems. The basic method is one that has been previously suggested in the narrower context of an application of distribution fitting involving a geological problem [8], but where the mathematical and statistical properties of the method were not established. We give some properties of the method and show that under general conditions it will identify the correct model asymptotically. An outline of the method is as follows.

2 METHOD

We suppose that there exists data, X, drawn from the unknown true system; so that the output from our simulation model can be compared with this. Our basic method is to allow for several, K say, competing models with probability distributions $F_i(\cdot, \theta_i)$ $i = 1, 2, ..., K.$, where the θ_i are unknown parameters, and

combine them as a *finite mixture* model:

$$F(\cdot,\theta) = \sum_{i=1}^{K} \alpha_i F_i(\cdot,\theta_i)$$

where $\sum_{i=1}^{n} \alpha_i = 1$, and $\alpha_i \geq 0$, $i = 1, 2, .., K$. Thus the F_i are treated as *components* of a mixture model. The full model is identified by finding which α_i's are non zero. For simplicity we consider only the hierarchical case, where, if the kth ($k < K$) component is included, then all components $k-1$, $k-2$, ..., 2, 1 are also included. The problem is then simply to select k. A sequential procedure is easily applied in this case by adding components successively to the model. At stage k, the model with k components is fitted to the true data, X, and for this fit, the value t, of an appropriately selected goodness-of-fit test statistic T, is calculated. Also at this stage, the distribution of the statistic T is calculated by parametric bootstrapping, assuming the fitted k component model is the correct one. The next stage is entered if t, as calculated from X, indicates the fit of this model to be significantly poor.

One of the advantages of the method is that there is a free choice as to the test statistic used. In classical methods, test statistics known to be sensitive for detecting certain kinds of lack-of-fit, such as a poor fit in the tails, are hard to work with in practice because their distributional properties vary depending on the model being fitted. The situation is exacerbated by the fact that these distributional properties depend on whether parameters of the distribution have to be estimated or not. For example the Anderson-Darling test statistic is designed to be sensitive to departures in the tails, but critical test values alter significantly if the parameters have to be estimated. One of the reasons why a demonstrably less sensitive test, such as the Kolmogorov-Smirnov test, remains popular is the fact that its distribution is not dependent on the model being fitted, at least when parameters do not have to be estimated.

In contrast, the bootstrap method suffers no such difficulties, because its distribution is actually computed *in situ*, so there is no need to worry about this, and the choice of test statistic can be focused purely on whether it is sensitive or not.

3 EXAMPLES

We give three examples. The first involves the study of the motion of stellar populations in a galaxy. We analyse a large data set given in [9]. The existence of three stellar populations is well known, and our analysis shows that the above bootstrap method does indeed corroborate this.

The second example is a data set giving the enzyme activity in blood in 245 unrelated individuals. The data was analysed in [10], and reanalysed using Bayesian methods in [7]. According to the Bayesian analysis there appears to be evidence for 3 or 4 components if a mixture model is fitted. We analyse the data and come to a more parsimonious conclusion that the data are capable of being explained by a model with fewer components.

The final example is a sample of measurements of an acidity index in 155 lakes in north-eastern USA. This data set was analysed in [11], and also analysed in [7] using Bayesian methods. We use the above bootstrap method to reanalyse this data set. Again our conclusion is that rather fewer components are needed than appears to be suggested by the Bayesian analysis.

4 CONCLUSIONS

The suggested bootstrap method gives an easy to apply method for model selection in problems where the dimensionality is not known. The method is very flexible, allowing great freedom in choice of test statistic used to determine the goodness-of-fit. Thus priority can be given to selecting a statistic that is especially suited for the given problem, without the worry that the statistic will be hard to work with because its distribution is difficult to determine.

In the examples given there is evidence that the method points to more parsimonious models than that given by Bayesian analysis.

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A COMPARISON OF METHODS FOR CALCULATING CONFIDENCE INTERVALS FOR SIMULATION OUTPUT

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1 INTRODUCTION

Output from a simulation model is subject to two sources of variability. There is inherent variability caused by the use of random number generators within the model (simulation variability). There is also, in the case of models dependent upon unknown input parameters, variability due to the estimation of those unknown parameters (parameter variability). Cheng and Holland [1,2,3] have discussed four methods for estimating total variability in a measure of simulation output.

2 METHODS

The first of these methods is based on the classical method of statistical differential analysis (often called the δ-method). The disadvantage of this method is that the computational effort increases linearly with the number of unknown parameters. The second method is based on bootstrap methodology. Although in many cases the bootstrap is computationally inefficient, in comparison with the δ-method for cases where there are a large number of unknown parameters, it can be competitive. The third method is based on the δ-method, but is modified so that the combined effect on the response output of variation in all the parameters is assessed by making simulation replications at just two settings of parameter values. We refer to the method as the δ/Two-Point method. The fourth method is referred to as the simplified Two-Point method, and essentially places all computational effort into simulation replications at the two settings of the parameter values.

In this paper, we take the four methods and apply them to estimation of confidence intervals. For the δ-method, we use standard normality theory in forming the confidence interval directly from an estimate of the variance. Similarly, for the δ/Two-Point method the estimate of variance may be used to construct confidence intervals. However, in bootstrap theory, there are three methods outlined for estimation of confidence intervals. These are the percentile method, the studentized method and the accelerated bias corrected percentile (BC_A) method. Results for the Bootstrap experiments were not available at the time of writing and will be presented later. For the simplified Two-Point method, the spacing between the two settings of the parameter values may be adjusted so that a confidence interval is calculated directly by the difference observed in the simulation output at the two points.

3 APPLICATIONS

The approaches outlined above are illustrated by consideration of two applications. Firstly, we consider an application taken from Chang et al. [4]. The situation is one of a communications switch with a finite buffer, fed by a number of sources. The measure of interest is the probability of buffer overflow. The model is based on a single switch, such as an ATM (Asynchronous Transfer Mode) communications switch, that can be sent traffic from K independent sources. The buffer size of the switch is B, and the switch can process up to c packets per time unit. The arrival streams are modelled via two-state Markov chains, where the two states correspond to either zero or one arrival per unit of time.

We consider a specific example consisting of 16 independent source nodes. We take $c = 8$ and $B = 10$. Each of the two-state Markov chains requires the two diagonal probabilities to be estimated by observation of traffic streams in the network. We take a sample of 10,000 observations from each data source in order to estimate these probabilities. Thus there are 32 estimated input parameters and thus for the δ-method, we require each simulation experiment to consist of 33 runs. For the δ-method, each run consisted of 1,000 subruns. Thus, there are 33,000 subruns in total. For the δ/two-point method, we need to choose an appropriate division of effort between the first and second stages. We consider instances where the simulation time is divided 50%-50%, 25%-75% and 10%-90%. In terms of subruns, this means that stage 1 and stage 2 consist of 500 and 8250, 250 and 12,375 and 100 and 14,850 subruns per simulation run respectively. For the simplified two-point method, each of the two runs consisted of 16,500 subruns. Table 1 gives estimates of confidence intervals and coverage obtained by the confidence intervals for the δ-method, δ/Two-Point method and the simplified Two-Point method. The important result to note here is that the simplified Two-Point method provides a very conservative upper bound on the confidence interval width. This has been achieved without evaluation of any differential coefficients but has cost exactly the same computational effort as the other two method. However, the conservative nature of this bound is dictated by the parameterisation of the simulation, and not the simulation effort employed. In other words, this bound can be calculated with significantly less computing effort than has actually been expended. To see this, we reproduce the simulation experiment for the simplified Two-Point method, but utilise only one tenth of the number of subruns. This experiment produces a confidence interval width of 9.0×10^{-3} and coverage of 100%, which is virtually identical to the full experiment. Thus the simplified Two-Point method provides an upper bound in a fraction of the computing effort that is required for either method that produces an actual estimate. Both of these methods suffer loss of accuracy when the simulation time is reduced.

Table 1 90% Confidence Interval Width and Percentage Coverage Obtained by δ-method, δ/Two-Point method and simplified Two-Point method for ATM Switch model.

Method	*C.I.Width*	*Coverage*(%)
$\delta - method$	1.7×10^{-3}	94
$\delta/Two - Point\, method\,(50\% - 50\%)$	1.5×10^{-3}	90
$\delta/Two - Point\, method\,(25\% - 75\%)$	1.4×10^{-3}	83
$\delta/Two - Point\, method\,(10\% - 90\%)$	1.6×10^{-3}	83
$simplified\ Two - Point\, method$	8.7×10^{-3}	100

The second example is one of a computer communications network. The network consists of N nodes connected via M channels, each of which receives packets of information from external and internal sources. We take $N = 10$ and $M = 11$. The $i'th$ communication channel has a capacity of C_i bits per second. The $j'th$ node has nodal processing time of K_j. Traffic entering the network at node l destined for node p forms a Poisson process with mean messages per second of γ_{lp}. The length of each message is also a Poisson random variable with mean $1/\mu$. We assume that there is no limit on nodal storage capacity and that message follow fixed paths through the network. Clearly, transmission time of messages from node to node is also dependent on the length of the channel (l_i for channel i). We are interested in estimating mean overall delay in the network. It is clear that this model possesses a large number of variables. Some, such as C_i and l_i should either be known exactly or we should be able to accurately estimate them. However, $\gamma_{lp}$and $1/\mu$ can only be estimated by observation of samples of values. We consider an example where $K_j = 1 \times 10^{-5}$ seconds ($j = 1, ..., 10$), $C_i = 15$ Mbytes/second and $l_i = 10$ miles ($i = 1, ..., 10$) . The γ_{lp} and $1/\mu$ were estimated from samples of 1000 observations. As there are $p = 91$ parameters and 100 subruns are performed per run, the total number of subruns implemented for the δ-method was 9200. If identical percentage divisions to the previous example were utilised between stage 1 and stage 2 for the δ/Two-Point method, then the number of subruns per run in stage 1 and stage 2 would be 50 and 2300, 25 and 3450, and 10 and 4140. Similarly, for the simplified Two-Point method 4600 subruns for each of the two runs would be available. However, due to the computational intensity of each simulation run, the number of subruns implemented in each second stage run was limited to 1000. Thus, each Two-Point experiment provides a computational saving over the δ-method, as shown in Table 2.

Table 3 gives 90% confidence interval and actual coverage obtained results. The advantage of the δ/Two-Point method over the δ-method is clearly visible. Again, the simplified Two-Point method provides a conservative bound on the confidence interval. Though the confidence interval width is almost three times that provided by the δ-method, the computational time required by the δ-method is over 4.5 times greater. Also, as mentioned earlier, no differential coefficients were estimated, making the implementation of the method very straight-forward.

Table 2 Computational Workload Required for Calculation of 90% Confidence Interval Width and Percentage Coverage Obtained by δ-method, δ/Two-Point method and simplified Two-Point method for Communications Network

Method	*Number of Subruns Performed*
$\delta - method$	910,000
$\delta/Two - Point\ method\ (50\% - 50\%)$	655,000
$\delta/Two - Point\ method\ (25\% - 75\%)$	427,500
$\delta/Two - Point\ method\ (10\% - 90\%)$	291,000
$simplified\ Two - Point\ method$	200,000

Table 3 90% Confidence Interval Width and Percentage Coverage Obtained by δ-method, δ/Two-Point method and simplified Two-Point method for Communications Network

Method	*C.I.Width*	*Coverage(%)*
$\delta - method$	4.06×10^{-3}	91
$\delta/Two - Point\ method\ (50\% - 50\%)$	3.90×10^{-3}	91
$\delta/Two - Point\ method\ (25\% - 75\%)$	4.00×10^{-3}	92
$\delta/Two - Point\ method\ (10\% - 90\%)$	4.15×10^{-3}	90
$simplified\ Two - Point\ method$	1.20×10^{-2}	100

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INFLUENCE OF THE PRODUCTION PROCESS TOLERANCES ON THE QUALITY OF SQUIRREL CAGE INDUCTION MOTORS

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1 INTRODUCTION

The dispersion of the output parameters of mass produced electrical machines is the natural effect of : deviations of the physical features of the applied row materials , deviations of the geometrical dimensions of the produced elements and the production process changes. The deviation of the output parameters is , in case of small electrical machines , one of the most important aspects of their quality since they are produced in large quantities and a high level of standardization of the output parameters and the main dimensions (particularly in case of low voltage cage induction motors) has been imposed . Therefore the sensitivity of electrical machines to the inaccuracy of the manufacturing process and the uniformity of their output parameters can be regarded as one of the measures of their quality .The determination of the role of particular input variables in the creation of the output parameters dispersion can lead to the strong limitation in the number of variables which are to be controlled and verified during the production process. The problem becomes even more complex when we take into account fact that the number of input and output parameters of electrical machines is substantial and their contribution to the machine's quality is usually different. This has created a demand for new quality measures which would be capable of selecting the most important input variables the scatter of which influences at most the quality of the whole series of mass produced product characterized by a number of different output parameters. The aim has been achieved basing on the Sensitivity Analysis .

2 BASIS OF THE ANALYSIS METHOD

The parameters of electrical machines are functions of geometrical dimensions and physical properties of materials used in the constructions. Deviations of these quantities, to be subsequently called input quantities, depending on their interaction and statistical distribution, can in a different way influence the value of the end parameter. In mass production, which is a stochastic process, we may assume that all input quantities (or input variables) are independent and that their distribution is close to the normal. In such a case the relation between the variation of parameter $Y= f(X_1...X_i...X_n)$ and the variation of input parameters X_i can be written as:

$$(\gamma_Y)^2 = \sum_{i=1}^{n} (\alpha_i \gamma_i)^2 \qquad (1)$$

where:

- γ_Y - variation coefficient of parameter Y,. $\gamma_Y = \frac{\sigma_Y}{Y}$, σ_Y - standard deviation;
- γ_i - variation coefficient of input quantity X_i , $\gamma_i = \frac{\sigma_i}{X_i}$, σ_i - standard deviation;
- α_i - influence factor of input parameter X_i : $\alpha_i = \frac{\partial f(X_i \ldots X_n)}{\partial X_i} \frac{X_i}{Y}$ (2)

Analyzing equation (1) and (2), with known input quantity scatter parameters, one can determine the scattering of the end parameter Y and find the contribution of the individual input quantities to this scattering. The function describing the dependence of a given parameter of an electrical machine on technological and constructional quantities has usually a very complex form and number of input quantities in considerable. The presented method of sensitivity analysis first applied in mechanics was known also as Dimensional Chains of Physical and Geometrical Quantities [4]. The method has been successfully adopted to investigations of electrical machines quality [2,7].

3 QUALITY COEFFICIENTS

In order to give more general information referring to the whole series of investigated machines and the larger number of their output parameters as well as to select the input variables determining either the dispersion of the particular output parameter but seen from the point of view of the whole series , or the quality of the whole series of investigated motors , the normalized quality coefficients have been introduced [2].
a/ normalized dispersion of the output parameter:

$$\beta_{jk} = \frac{3\sigma_{jk}}{B_{jk}} \tag{3}$$

where:

- j - number of the output parameter
- k - number (type) of motor
- σ_{jk} - standard deviation of the output parameter calculated with the help of the Sensitivity Analysis
- B_{μ} - reference tolerance

Such a kind of normalization has its background in case of investigation of a production process capability - described in [5]
b/ In order to compare the quality of different types of motors, with respect to their output parameters scatter, an average normalized scatter coefficient has been introduced:

$$D_k = \frac{1}{j}\sum_{1}^{j}\beta_{jk} \tag{4}$$

This measure has allowed for comparison of scattering of different output parameters of mass produced machines
In order to assess the role of particular input variable in the final quality of investigated machines a set of partial normalized quality coefficients has been proposed [2,3] and implemented.

1/ d_{ij}^{k} - normalized percentage content of the i-th input quantity deviations in the scatter of the j-th parameter of the k-th motor:

$$d_{ij}^{k} = \frac{(\alpha\gamma)_{ij}^{2k}}{\sum_{i=1}^{n}(\alpha\gamma)_{ij}^{2k}} \times \beta_{jk}^{2} \times 100\% \tag{5}$$

The above coefficient has allowed for the quantitative comparison of the influence on different input variables on the quality of the k-th motor.

2/ Normalized partial coefficient - d_i^k

$$d_i^k = \frac{1}{j}\sum_{j=1}^{j} d_{ij}^{k} \tag{6}$$

The coefficient determines the percentage content of the i-th input variable on the average reference deviation of all (j) taken into account output parameters in case of a particular k-th type of motor. It is a measure of the influence of the i-th variable scatter on the quality of the k-th motor type.

3/ Normalized partial coefficient - d_{ij}

$$d_{ij} = \frac{1}{k}\sum_{k=1}^{k} d_{ij}^{k} \tag{7}$$

The coefficient has allowed for the quantitative determination of an influence of an i-th input variable scatter on the final dispersion of the chosen (j-th) parameter within the whole series of k types of machines.

4/ In order to determine the variables which play a decisive role in the creation of the quality of the whole series of investigated machines the normalized coefficient d_i has been proposed.

$$d_i = \frac{1}{k}\sum_{k=1}^{k}\frac{1}{j}\sum_{j=1}^{j} d_{ij}^{k} \qquad (8)$$

The coefficient determines the influence of the i-th input variable on the quality of k - types (whole series) motors with respect to deviations of their j (taken into account) output parameters.

4 PRACTICAL IMPLEMENTATION

Basing on the results obtained with the help of Sensitivity Analysis (Dimensional Chains of Physical and Geometrical Quantities) and utilizing the proposed normalized quality coefficients a whole series (9 types) of three phase cage induction motors of low power have been investigated [1,6]. The rated power of investigated machines varies from 0.55 kW to 4 kW with the rated speed range from 670 to 2850 rpm. The chosen types of motors had been already produced for over 5 years so the production process could be regarded as the stabilized one. The yearly production rate of each motor type exceeded 10 thousand motors so that the production process could be regarded as a mass production.

The set of the chosen output parameters consisted of :

- No load current
- Starting torque
- Short circuit current
- Maximum torque
- Power factor at rated speed
- Efficiency at rated speed
- Temperature at full load

Number of input variables varies from 23 to over 100 depending upon the output parameter

As a result a group of only few input variables, out of over 100, have been selected. These are:

- Variables determining rotor and stator windings resistance: conductivity of the rotor's cage and stator winding , average length of a stator winding turn and the diameter of a stator copper wire.
- Variables determining the motor air-gap : stator bore and rotor outer diameter
- Variables the scatter of which influences rotational losses - this refers mainly to a bearing and a bearing shield
- Influence of the magnetic properties of the applied steel sheets and the applied insulation materials were also not negligible however their role was not the most significant in the creation of the overall quality of the investigated machines with respect to the taken into account output parameters.

The above listed variables determine in more than 90% the quality of the whole series of the investigated motors (from the point of view of the dispersion of the investigated output parameters).

CONCLUSIONS

The implementation of the quality coefficients allows also the comparison of different types of motors from the point of view of their output parameters dispersion , and the comparison of the role of variations of different input variables according to their influence on the quality of the investigated motors. The variables determining the quality of induction motors (from the point of view of the average dispersion of their output parameters) as well as the variables determining the dispersion of a particular output parameter (from the point of view of the whole series of investigated motors) have been selected.

The presented method can find a wide application in the quality control of any mass produced device determined by a large number of input variables and characterized by a number of different output parameters.

The same refers to the whole series of electrical devices of similar construction.

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MISSING DATA PROBLEM AND KALMAN FILTER: A CASE STUDY ON ENVIRONMENTAL DATA

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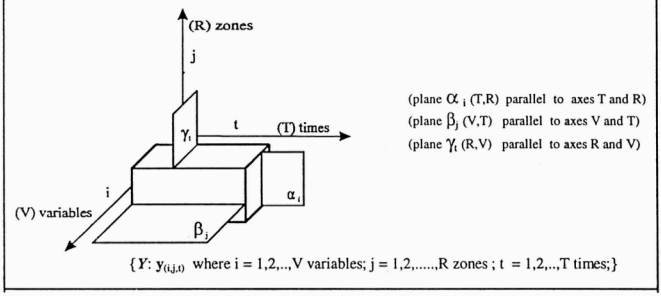
Summary: This paper proposes a method for the reconstruction of missing data in a three way data matrix, based on modified procedures of the optimum Kalman filter in relation to the structural data analysis. The case study take a look at some environmental data on sea water pollution observed in the Adriatic sea.

Key Words: Kalman filter, state-space model, missing data, three way environmental data matrix.

1 INTRODUCTION

The aim of this paper is to propose a methodology for the reconstruction of missing data in a three way matrix, supposing that the environmental observations, $y_{(i,j,t)}$, characterised by three co-ordinates: type of variables, space and time, are represented through a dynamic system in state-space.
The above mentioned representation based on particular Markovian stochastic processes, consents the change of state from past information to future information through an optimum filtering proposed by R.E. Kalman, already adopted in the past to study the modern system theory (Kalman and Bucy, 1960).
Such a dynamic system results completely specified if it is structured in terms of two equations, where the first, namely of transition or state equation, shows the functional composition of the state parameter, while the second equation, namely of observation, tries to forecast the future observations or, as in our case, to reconstruct the missing information.

fig. A Exemplification of three way data matrix object of study.



Based on our knowledge of this topic, the problem of missing data on three-way matrices, was not studied univocally and nor were proposed methods or techniques valid for any case study. The most frequently adopted techniques utilise methods used in time series analyses, linked to ARIMA class models, of which its application is restricted by stationary and isotropic conditions, as well as equally spaced units of measurements of the variables.

2 THE MODEL

Any interpretative dynamic model of three-dimensional data, should be able to reproduce, with its own structure, the interrelationship of the variables in any of the three directions of the system.In particular to analyse a phenomenon characterised by a set $\{Y: y_{(i,j,t)}$ where i = 1,2,..,V variables; j = 1,2,.....,R zones ; t = 1,2,..,T times;$\}$the three way matrix can be completely reconstructed in its missing parts through a procedure that requires the collapse of one or two dimensions (fig. 1).

Choosing, for example the i-th variable, the corresponding plane α_i(T,R), parallel to axes T and R, is a space-time matrix, where it is possible to apply the bidimensional optimum Kalman filter, to reconstruct the missing data.

Analogously choosing, the j-th zone, the corresponding plane β_j(T,V) parallel to axes V and T, identifies a matrix containing a multiple time series, on which it is possible to apply the Kalman filter for autoregressive vectorial models (VAR).

In our paper, we intend to propose six procedures. Four are based on a bidimensional Kalman filter, and two are based on the ordinary Kalman filter, in which, the first is an ARIMA model and the second is an autoregressive vectorial model. Moreover, for some of these procedures, those whose names include the letter S, we have applied the smoothing algorithm.

From the above considerations, a flexible and general approach for the reconstruction of missing data in a three way matrix can be carried out considering a linear model of two vectorial equations. The first, said state equation, is $\mathbf{X}_{s+1} = \Phi\mathbf{X}_s + \mathbf{W}_{s+1}$,while the second said observation equation, is $\mathbf{Y}_s = \mathbf{A}^T\Psi + \mathbf{H}_s\mathbf{X}_s + \mathbf{V}_s$, where Φ $\mathbf{H}$ and $\mathbf{A}^T$ are matrices of parameters matrix; $\mathbf{W}_s$ e $\mathbf{V}_s$ are observations and state Gaussian zero mean noises with covariances equal to Qw and Qv; Ψ is a vector of exogenus or predetermined variables. In such terms, the Kalman filter can be expressed through two phases: forecasting and updating for to determine the optimal estimate of the state vector X_s, whenever new information becomes available. The optimal estimate of $\mathbf{X}_{s+1}$ is given by: $\hat{\mathbf{X}}_{s+1/s} = \Phi\hat{\mathbf{X}}_{s/s}$ while the covariance matrix of the forecast error is $\mathbf{P}_{s+1/s} = \Phi\mathbf{P}_{s/s}\Phi' + \mathbf{Q}_w$. These two equations are known as forecasting equations. Once the new information $\mathbf{Y}_s$, becomes available the estimate $\hat{\mathbf{X}}_{s/s}$, can be updated. The updating equations are: $\hat{\mathbf{X}}_{s/s} = \hat{\mathbf{X}}_{s/s-1} + \mathbf{K}_s\left[\mathbf{Y}_s - \mathbf{H}\hat{\mathbf{X}}_{s/s-1}\right]$ and $\mathbf{P}_{s/s} = \left[\mathbf{I} - \mathbf{K}_s\mathbf{H}_s\right]\mathbf{P}_{s/s-1}$ where $\mathbf{K}_s$ is the Kalman gain matrix.

In some cases the state vector can be interpreted in structural terms, so it is more appropriate to estimate its value at a particular point, using all the information and not just a part of it.

Such an inference is called the smoothed estimate while the corresponding estimator is called smoother. Since the smoother is based on more information than the filtered estimator, it will have a mean squared error which, in general, is smaller than that of the filtered estimator.

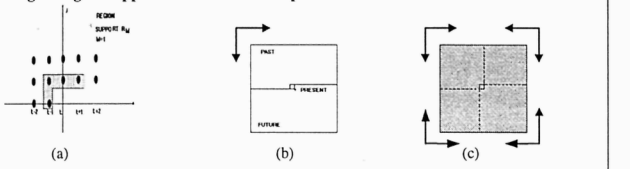
In statistical literature have been proposed several smoothing algorithms in linear models, and in our paper we will use algorithms known as fixed-interval and fixed-lag smoothing. The first algorithm is concerned with computing the full set of smoothed estimates for a fixed span of data and imply a backward recursion of the Kalman filter, the latter algorithm computes smoothing estimates for a fixed delay and runs in parallel with the Kalman filter (Anderson and Moore, 1979).

As we can see in fig. 1, the plane α_i(T,R) is referred to a space-time matrix associated to the i-th variable and we can apply the ordinary unidimensional or bidimensional Kalman filter method. In particular, when applying the bidimensional Kalman filter, we must resolve two types of problems: the first is associated to the dimension of the state vector and the second is related to the absence of a privileged direction.

To by-pass the high dimension of the state vector problem, the model for the reconstruction of the missing data that we propose, regards the Ordinary Reduced Kalman Filter (ORKFS) (fig. 2.b). In this case, the updating procedure is based on a limited number of information near the generic observation $y_{\alpha_i}(j,t)$ on plane α of the i-th variable at the t-th instant and in the j-th zone as indicated in (fig. 2a).

As far as the second problem is concerned, since in our case it is necessary to give the filter a direction, we will assume that the updating is done starting with the upper left axis, moving along observations from left to right and row after row (Woods, 1977) (fig. 2.b).

fig. 2 Region support and restriction dependence of FKRO and FKMO



(a) (b) (c)

The ORKFS requires the specification of one region of support R_M (fig.2.a), where the updating procedure of the estimate of the state vector will be realized.
The region R_M is defined by the following equation:

$$R_M(j,t) = \left[(t-g, j-h) \middle| (1 \le h \le M; 0 \le g \le M) \cup (-M \le h \le 0; 1 \le g \le M)\right]$$

where M =1,2 defines the recursive model order.
This allows us to define the generic elements $y_{\alpha_i}(i,t)$ through the following state equation:

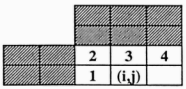
$$x_{\alpha_i}(j,t) = \sum_{(j-h;t-g)\in R_M} \phi_{hg} x_{\alpha i}(j-h, t-g) + w(j,t)$$ where ϕ_{hg} represents the coefficients that regulate the relation

between $x_{\alpha i}(j,t)$ and $x_{\alpha i}(t-g;j-h)$ and w(j,t) is the realisation of a Gaussian stochastic field previously defined. In such a contest, a bidimensional Kalman filter can produce both filtered estimate and fixed lag smoothed estimate.
Since the implementation of the ORKFS requires the coupling coefficient vectors ϕ and the process noise variance σ^2, the autocorelation function is used to identify these quantities directly from the data (as suggested by H.Kaufman, J.Woods etc, 1983):

$$\sum y_{\alpha_i}(i,t) y_{\alpha_i}(i-k, t-l) = \phi' \sum \left(\mathbf{y}_{\alpha R_M}\, y_{\alpha}(i-k, t-l)\right) \qquad (1)$$

where:
- $\mathbf{y}_{\alpha RM}$ is a vector consisting of those data in R_M region related to the zone considered by the sum operator.

Collect the data $y_{\alpha_i}(i,t)$ over a representative data block L and choiced a support region containing the observation at lag (k,l), it is possible, assuming the invertibility, to solve (1) for ϕ directly or by a least-square fit. Many experiments realized for several values of k and l, have suggest the following correlation region represented by the shadowed area:



Once obtained the estimate of the parameter vector, it is possible to estimate the process noise variance as follow

$$\hat{\sigma}^2 = \frac{1}{N_L} \sum \left(y_{\alpha i}(i,t) - \hat{\theta}' \mathbf{y}_{R_M}\right)^2$$

where:

- N_L is the number of observation contained in the block L;

By changing the dependence restrictions, the ORKFS procedure (fig. 2.b.), can be repeated starting from each vertex of the plane. The final estimate of the missing data is an average of the obtained results. This new procedure is a modification of the ORKFS and has been called the Ordinary Modified Kalman Filter (OMKFS) (fig. 2.c).

Keeping in mind plane $\alpha_t(T,R)$, an alternative procedure called RWKS (Reduced Weighted Kalman Filter and Smoothing), consists in highlighting an eventual recurring data structure, for example a seasonal index, useful for weighting the estimates obtained with the ORKFS procedure.
The last two proposed procedures require an univariate and multivariate time series analysis. Particularly, on plane $\alpha_t(T,R)$, we can identify a time series for each zone and utilise the ordinary Kalman Filter for ARIMA class models (FKARMAS). On the contrary, on plane $\beta_t(V,T)$ we can filter with an autoregressive vectorial model (VAR), which has been called FKVARS.

4 THE CASE STUDY

The data of this study, are related to the results of a monitoring project and concerns the presence of some polluting substances held responsible for the Eutrophications phenomenon. The cubic matrix proves to be defined by 10 variables, 17 zones and 49 times. From the above mentioned matrix, several observations were voluntarily eliminated in such a way as to internally obtain a "cloud" of missing data. This cloud was then reconstructed using the six adopted procedures and the goodness of fit was evaluated using the R squared measure. The following tables show the measure and ranks of the R square, calculated for our first five procedures for each of the ten observed variables. In our case study, the method that best furnished the lowest R squared values is the MRWKF.

Tab 1. Values of R square calculate for the first five procedures for each of ten variables

	Variables									
Procedures	1	2	3	4	5	6	7	8	9	10
ORKFS	0.90	0.95	0.90	0.93	0.96	0.92	0.90	0.96	0.97	0.90
OMKFS	0.95	0.89	0.95	0.92	0.95	0.95	0.91	0.90	0.94	0.86
RWKF	0.91	0.78	0.92	0.91	0.72	0.97	0.97	0.94	0.90	0.92
MRWKF	0.87	0.84	0.91	0.89	0.90	0.99	0.95	0.96	0.98	0.97
FKARMAS	0.92	0.93	0.87	0.85	0.68	0.90	0.86	0.83	0.88	0.84

Tab 2. Ranks of the R square obtained with each of the five procedures

	Variables											
Procedures	1	2	3	4	5	6	7	8	9	10	Average	Ranks
ORKFS	4°	1°	4°	1°	1°	4°	4°	1°	2°	3°	2.5	2°
OMKF	1°	3°	1°	2°	2°	3°	3°	4°	3°	4°	2.6	3°
RWKF	3°	5°	2°	3°	4°	2°	1°	3°	4°	2°	2.9	4°
MRWKF	5°	4°	3°	4°	3°	1°	2°	1°	1°	1°	2.4	1°
FKARMAS	2°	2°	5°	5°	5°	5°	5°	5°	5°	5°	4.2	5°

This means that the previous exploration data analysis, and thus, the consideration in the model of information characterizing the data structure composition, have been very important to obtain the best reconstruction of the missing data.
As demonstrated in the table below, even the last procedure using the VAR, which was called FKVARS, shows in the presence of a multiple time series, a satisfying reconstruction capacity of missing data.

Tab. 3 R square obtained using the FKVAR procedure

	Zones with missing data							
	7	8	9	10	11	12	13	14
Rsquare	0.89	0.91	0.93	0.94	0.79	0.97	0.91	0.86

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LOCAL PROBABILISTIC IMPORTANCE MEASURES FOR COMPARING FORM AND MONTE CARLO CALCULATIONS ILLUSTRATED WITH DYKE RING CALCULATIONS

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1 INTRODUCTION

The Dutch government is currently undertaking an extensive study of dyke ring reliability, with uncertainty. The reliability of dyke section i is expressed in terms of a reliability function

$$Z_i = \text{Strength}_i(X_{i1}, \ldots X_{in}) - \text{Load}_i(X_{i1}, \ldots X_{in})$$

where strength and load are functions of uncertain parameters $X_{i1}, \ldots X_{in}$. The reliability for a dyke ring consisting of K dyke sections is

$$Z = \min = \{Z_1, \ldots Z_K\}.$$

The example discussed below involves one failure mechanism, overtopping and some 300 uncertain parameters. Since all dyke sections are exposed to the same sea water levels, the same river discharges and the same winds, there are significant dependencies in the reliabilities of different dyke sections Monte Carlo (MC) and First Order Methods (FORM) have been used with an 'in house' assessment of uncertainty for the purpose of comparing the dependency modeling and comparing the relative importances of various input parameters.

2 FORM

Suppose $Z(X_1, \ldots X_n)$ is a 'deterministic' function of random variables $X = X_1, \ldots X_n$. Assuming that Z is analytic, we can linearize it about some point $x^* = x_1^*, \ldots x_n^*$:

$$Z(X) = Z(x^*) + \sum (X_i - x_i^*)\partial_i Z(x^*) + \ldots \text{ HOT (higher order terms)},$$

where ∂_i denotes $\partial/\partial x_i$. x^* is chosen as the "design point", that is the point with greatest probability density satisfying $Z(x^*) = 0$.

Let μ_i and σ_i denote the mean and standard deviation of x_i, respectively. Neglecting the HOT's, we have

$$\begin{aligned} Z(X) &= Z(x^*) + \sum (X_i - x_i^*)\partial_i Z(x^*) \qquad (1 \\ E(Z) &\sim Z(x^*) + \sum (u_i - x_i^*)\partial_i Z(x^*); \\ \text{Var}(Z) &\sim \sum \sigma_i^2 (\partial_i Z)^2 + \sum \partial_i(Z)\partial_j(Z)\,\text{COV}(X_i, X_j); \end{aligned}$$

and if the X_i's are all independent, $\text{Var}(Z) \sim \sum \sigma_i^2 (\partial_i Z)^2$.

Now suppose that Z is indeed linear and the X_i's are indenpendent. Then

$$COV(Z, X_i) = \rho(Z, X_i)\sigma_Z \sigma_i = \partial_i Z COV(X_i, X_i) = \sigma_i^2 \partial_i Z$$

so that

$$\rho(Z, X_i)\sigma_Z/\sigma_i = \partial_i Z(x^*). \quad (2)$$

Note that the LHS involves "global" parameters, whereas the RHS depends on the design point x_i^*. It is characteristic of linear models that these global and local concepts coincide. $\rho(Z, X_i)$ is taken to represent the importance of X_i for Z. Note that in the FORM model this has both a global and a local interpretation.

Continuing,

$$\sigma_Z^2 = \sum \sigma_i^2(\partial_i z)^2 = \sum \rho^2(Z, X_i)\sigma_Z^2; \text{ or}$$

$$R^2 = \sum \rho^2(Z, X_i) = 1.$$

In the terminology of linear models $R^2 = \sum \rho^2(Z, X_i)$ is the percentage of the variance of Z that is explained by the linear model (1). If R^2 is less than one, this may be caused *either* by dependencies in the X_i's or by contributions from HOT's in (1).

Several authors[1] propose the correlation ratio CR_i to replace $\rho(Z, X_i)^2$ for cases when Z is not linear:

$$CR_i = \text{VAR}(E(Z|x_i))/\text{VAR}(Z)$$

Note that CR_i generalizes the global interpretation of importance in (2), but not the local interpretation. Moreover, CR_i cannot be computed in a straightforward way by MC methods.

3 HOW LINEAR IS Z_i?

For dyke section i, Z_i is computed from a model involving many cut-offs, edges, and non linearities. Nonetheless, because if its complexity, the question 'how linear is Z_i?' —cannot be answered by inspection. Using the MC calculation for section i, we can assess the linearity of Z_i simply by computing R^2. Curiously, we find $R^2 = 0.977$, with the largest contribution 0.903 coming from one variable (a 'strength model factor'). This does not correspond at all to the partial derivatives computed at the design point, which were dominated by the North Sea level. On the other hand, performing a conditional R^2 near the region of greatest failure probability we find (i) that the conditional correlations are sensitive to *how* the conditionalization is performed, and (ii) the conditional R^2 is quite small, though still dominated by the globally dominante parameter. This strongly suggests that Z is globally linear, as it is dominated by one variable, but in the region of interest, $Z \sim 0$, which has very low probability mass, Z's behavior is highly non linear. For this reason it is difficult to interpret the FORM importance parameters in terms of (conditional) correlations from a MC calculation.

4 LOCAL PROBABILISTIC IMPORTANCE

Suppose we are interested in the importance of variables in the region $Z \sim 0$. Consider

$$E(X_i|Z = 0).$$

If X_i were independent of Z, then this conditional expectation would be simply $E(X_i)$. If $X_i = Z$, then clearly $E(X_i|Z = z) = z$. This suggest the local probabilistic importance measure probabilistic importance measure

$$\partial E(X_i|Z = z)/\partial z_{|z=0}.$$

The following proposition relates this measure to the partial derivatives of a FORM linear approximation:

PROPOSITION; Let $X = X_i, \ldots X_n$ be independent standard normal variates and let

[1] McKay, M.D. (1977) "Nonparametric variance-based methods of assessing uncertainty importance" RESS vol 57 no 267-280

$$Z = \sum \alpha_i X_i;$$

then $X|Z$ is normal with

$$E(X_i|Z = z) = z\alpha_i/\ell^2;$$
$$\text{Var}\,(X_i|Z = z) = (\sum_{j\neq i} \alpha_j^2)/\ell^2;$$
$$\rho(X_i, X_j) = -\alpha_i\alpha_j/((\sum_{k\neq i} \alpha_k^2)(\sum_{k\neq j} \alpha_k^2))^{\frac{1}{2}}$$

where $\ell^2 = \sum \alpha_i^2$•

Assuming that the linear model (1) holds, with $(X_i - x_i^*)/\sigma_i$ independent standard normals, then $\alpha_i = \partial_i Z$ and it follows that

$$\partial E(X_i|Z = z)/\partial z = (\alpha_i\sigma_i^2/(\sum \alpha_i^2\sigma_i^2) = \rho(Z, X_i)\sigma_i/\sigma_Z.$$

Hence in the case of linearity, this local probabilistic importance measure agrees with the FORM measure. However, if linearity does not hold,

$$(\partial E(X_i|Z = z)/\partial z)\sigma_Z/\sigma_i$$

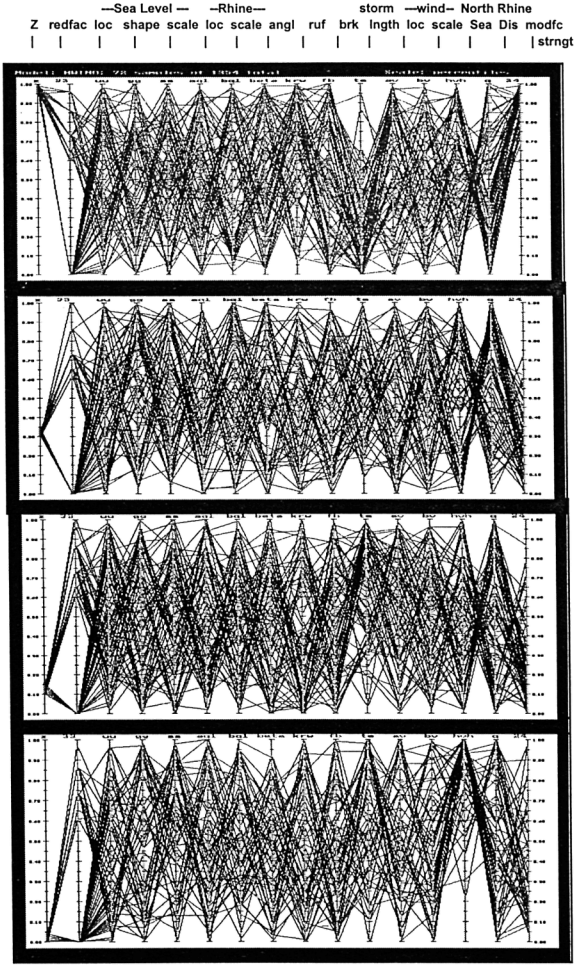
can be used to capture the local interpretation of (2), and it can be easily computed in MC calculations.

5 SOME RESULTS

Percentile cobweb plots show the joint distribution, in percentiles, of Z and 15 explanatory variables. Each vertical line represents one variable and each broken line represents one sample, intersecting each vertical line in the appropriate percentage point. This data is obtained by first conditionalizing on high, but not critical, sea and river water levels, giving 1354 samples. In 2% of these samples the dyke ring actually fails corresponding to the lowest 2% of the variable Z. These 1354 samples are uniformly distributed over all vertical lines (This graph is not shown). Four figures are shown, corresponding to conditionalizing on, from top to bottom, $Z \geq z_{95}, z_{35} \geq Z \geq z_{30}, Z_{15} \geq Z \geq Z_{10}$, and $z_{05} \geq Z$. Departure from uniformity indicates that conditionalization affects the distribution of the corresponding variable.

In the top graph the variables "storm lngth" and "modfc strngt" differ most strongly from uniform (redfac is a discrete variable). As we move down we see that first "storm lngth" then "modfc strngt" become more uniform, and North Sea becomes sharply non uniform for low Z values. The changes in conditional expectations accord the the FORM partials, with North Sea dominating in the region $Z \sim 0$.

Percentile Cobweb Plot for Dyke Ring Reliability, and Selected Input



EXPLOITING PROPERTIES OF SENSITIVITY ANALYSIS IN BELIEF NETWORKS

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1 INTRODUCTION

During the last decade *Bayesian belief networks* have become widely accepted as intuitively appealing representations of uncertainty that are highly valuable in addressing complex problems requiring a considerable amount of expertise for their solution. A Bayesian belief network basically is a concise representation of a joint probability distribution on a set of statistical variables [1]. It encodes, in a graphical structure, the variables of importance to the problem at hand, along with their probabilistic interrelationships; the strengths of these relationships are described by conditional probabilities. Successful belief-network applications presently concern, among others, medical diagnosis, prognostic assessment, and treatment planning [2].

A Bayesian belief network is generally constructed with the help of experts. Experience shows that building the graphical structure of the network is relatively straightforward. Assessing its conditional probabilities, however, is found to be a much more difficult task. Available techniques for the elicitation of well-calibrated probabilities from experts tend to be quite time-consuming and, in fact, have proved to be impracticable for assessing the usually large number of probabilities required. In practice, therefore, only rough assessments can be feasibly obtained.

Sensitivity analysis of a Bayesian belief network with rough, initial assessments serves to uncover the network's conditional probabilities for which the initial assessment suffices to arrive at satisfactory problem-solving behaviour and those for which a more accurate assessment is required. Sensitivity analysis thus provides for directing further elicitation efforts towards the most critical probabilities. We feel that a procedure of iteratively performing sensitivity analyses and refining probabilities will ultimately lead to a sufficiently robust network [3].

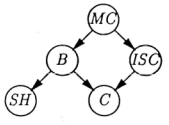
When performed straightforwardly, sensitivity analysis of a Bayesian belief network requires considerable effort. We have found, however, that the computational burden involved can be reduced by exploiting the relationships among the variables that are represented in the network. Conditional probabilities that can influence a probability of interest are readily distinguished from conditional probabilities that cannot, solely on the basis of the network's graphical structure and, hence, by qualitative arguments only. We in addition have found that the sensitivity of a probability of interest for a network's single conditional probability or pair of probabilities is described by a simple functional relationship. Making use of these properties provides for efficient sensitivity analysis of belief networks of realistic size.

2 BAYESIAN BELIEF NETWORKS

A *Bayesian belief network* basically is a representation of a joint probability distribution. It encodes, in a graphical structure composed of nodes and arcs, the variables of importance to a problem under study and the probabilistic relationships among them. Each node in this structure represents a statistical variable taking its value from a set of discrete values. The arcs in the structure represent probabilistic relationships among the represented variables: the tail of an arc indicates the cause of the effect at the head of the arc. Absence of an arc between two nodes means that the corresponding variables do not influence each other directly and, hence, are conditionally independent. The 'strengths' of the relationships among the variables are described by conditional probabilities: for each variable, the probabilities of its values are

specified, conditional on the various possible combinations of values for its immediate predecessors in the graphical structure. Figure 1 shows a small example belief network.

"Metastatic cancer (MC) is a possible cause of a brain tumour (B), and is also an explanation for increased total serum calcium (ISC). In turn either of these could explain a patient falling into a coma (C). Severe headaches (SH) are also associated with a brain tumour." [4]



$p(mc) =$	0.2	$p(c \mid b, isc) =$	0.8
$p(b \mid mc) =$	0.2	$p(c \mid \neg b, isc) =$	0.8
$p(b \mid \neg mc) =$	0.05	$p(c \mid b, \neg isc) =$	0.8
$p(isc \mid mc) =$	0.8	$p(c \mid \neg b, \neg isc) =$	0.05
$p(isc \mid \neg mc) =$	0.2		
$p(sh \mid b) =$	0.8		
$p(sh \mid \neg b) =$	0.6		

Figure 1: An example belief network representing a fragment of (fictitious) medical information pertaining to the presence of a brain tumour in an arbitrary patient.

The graphical structure and associated conditional probabilities of a Bayesian belief network with each other define a unique probability distribution. A belief network can therefore be used for calculating any prior or posterior probability of interest. Posterior probabilities are calculated by entering evidence into the network, that is, by entering the values for the nodes that are known, or are assumed to be known, with certainty. For calculating probabilities of interest, efficient algorithms are available [1,5].

3 SENSITIVITY ANALYSIS OF BELIEF NETWORKS

Sensitivity analysis is a general technique from the field of decision theory for studying the effects of the uncertainties in the parameters of a model on this model's outcome [6]. For a belief network, sensitivity analysis provides for example for studying the effects of the uncertainties in the network's assessments on a probability of interest. The simplest type of sensitivity analysis of a belief network is a *one-way sensitivity analysis* in which one of the network's conditional probabilities is varied within some plausible interval, keeping all other probabilities fixed. Such an analysis serves to reveal the effect of just the conditional probability that is being varied on a probability of interest. In a *two-way sensitivity analysis*, two conditional probabilities are varied simultaneously. In addition to the separate effects of variation of the two probabilities, a two-way sensitivity analysis reveals the joint effect of their variation on a probability of interest.

When performed straightforwardly, sensitivity analysis of a belief network requires considerable computational effort. In principle, every conditional probability of the network as well as every pair of probabilities is varied systematically; for each value and pair of values under study, the probability of interest is computed from the network. We have identified various properties that allow for increasing the efficiency of sensitivity analysis. In stating these properties, we will discriminate between two different types of state for a belief network: the network's apriori state and its aposteriori states. In the apriori state no evidence is available to the network, whereas in an aposteriori state for at least one node a value is known with certainty. Note that in an aposteriori state the network reflects a specific case or profile.

For a belief network under study, various one-way sensitivity analyses can be skipped due to their being *uninformative*, as their corresponding conditional probabilities are known to have no influence whatsoever on the probability of interest. These uninformative analyses are identified by inspection of the network's graphical structure and, hence, by qualitative arguments only. In the apriori state, the uninformative analyses are the ones that concern conditional probabilities for the variables for which there does not exist a directed path to the variable of interest in the network's structure. In an aposteriori state, at least all analyses concerning conditional probabilities for the variables that are separated from the variable of interest by the presence of evidence, are uninformative and can therefore be skipped.

From the probabilistic relationships represented in the graphical structure of a belief network, we further have found that a one-way analysis takes the form of a simple *functional relationship* between the conditional probability that is being varied and the probability of interest. In the network's apriori state,

a probability of interest $\Pr(V)$ depends *linearly* on the probability x that is being varied: $\Pr(V) = ax+b$, where a and b are constants. In an aposteriori state, the updated probability of interest $\Pr'(V)$ is a *reciprocal function* of the probability that is being varied: $\Pr'(V) = (ax + b)/(cx + d)$, where a, b, c, and d once more are constants. Figure 2 shows two one-way analyses for our example belief network, revealing the identified functional relationships.

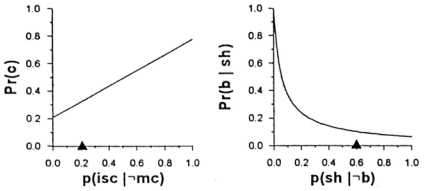


Figure 2: Two one-way analyses for the example belief network; the effects of variation of the conditional probabilities $p(isc \mid \neg mc)$ and $p(sh \mid \neg b)$ on the probabilities of interest $\Pr(c)$ and $\Pr(b \mid sh)$, respectively, are shown.

For two-way analyses of a belief network, similar functional relationships hold as for one-way analyses. In addition, while a two-way analysis may in general show a non-linear interplay of the conditional probabilities that are being varied, we have that, in a belief network's apriori state, a two-way analysis that involves probabilities conditional on at least one complementary value, reveals no unanticipated effects on a probability of interest beyond the effects shown by one-way sensitivity analyses for the two probabilities separately. Such an analysis therefore is uninformative and can be skipped. Figure 3 shows two two-way analyses for our example belief network, indicating a non-linear and a linear interplay of conditional probabilities, respectively.

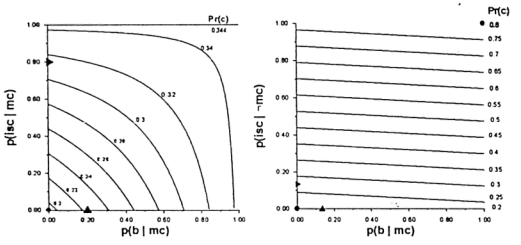


Figure 3: Two two-way analyses for the example belief network; the effects of simultaneous variation o $p(b \mid mc)$ and $p(isc \mid mc)$ and of $p(b \mid mc)$ and $p(ics \mid \neg mc)$, respectively, on the probability of interes $\Pr(c)$ are shown.

Making use of the properties outlined above allows for increasing the efficiency of sensitivity analysi of a belief network. Various one-way and two-way analyses can be skipped as they have been identifie as being uninformative. For the remaining analyses, determining the constants in the functional rela tionships suffices. These constants may be determined either by calculating the probability of interest fo several values of the conditional probability that is being varied and subsequently solving the resultin system of equations, or by computing the constants directly from the network. Further details will b provided in a forthcoming technical paper.

4 CONCLUSIONS

When building a Bayesian belief network, a large number of conditional probabilities will have to be assessed by experts. Although various techniques are available for the elicitation of well-calibrated probabilities, these techniques have proved to be impracticable for assessing all probabilities required. To allow for directing the elicitation efforts towards the most critical probabilities, sensitivity analysis can be performed on a network with rough, initial assessments. The computational burden involved in sensitivity analysis of a belief network, however, is considerable. We have discussed various properties that allow for increasing efficiency. By exploiting the graphical structure of a belief network, analyses that are worthwhile can be readily distinguished from those that are not. Furthermore, one-way and two-way analyses of a belief network obey simple functional relationships between the conditional probabilities that are being varied and the probability of interest. Determining the constants involved in these functional relationships therefore suffices. Making use of these properties considerably reduces the computational complexity of sensitivity analysis of a belief network of realistic size.

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APPLICATION OF THE FFT UNCERTAINTY QUANTIFICATION METHODOLOGY TO THE OECD-CSNI ISP-39

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ABSTRACT

The paper summarizes the accuracy quantification of the code prediction calculations carried out in the framework of the International Standard Problem 39 (ISP-39) using a methodology based on the Fast Fourier Transform (FFT) technique. ISP-39 is a code benchmark exercise organized by the Institute for Systems, Informatics and Safety (ISIS) of the European Commission (EC) Joint Research Center (JRC) in collaboration with the Committee on the Safety of Nuclear Installations (CSNI) of the Organization for Economic Cooperation and Development (OECD). The exercise was based on the Test L-14, a Fuel Coolant Interaction experiment performed in the FARO facility (JRC Ispra).

1 INTRODUCTION

The primary objective of ISP-39 [1] was the verification of the predictive capabilities of computer codes used in water cooled reactor severe accident progression analysis with particular attention to the simulation of molten fuel coolant interaction (MFCI) and quenching. As reference for the exercise were used the experimental results of a melt quenching test performed at JRC-Ispra in the FARO test facility; the test simulated the interaction of 125 kg of a molten UO_2ZrO_2 mixture (3000 °C) with a water pool saturated at a system pressure of 50 bar. Several research organizations from EC member countries as well as USA, Japan, Korea and Russia participated submitting calculations using 15 code or code versions (Table 1).

Table 1: ISP-39 Codes/Organizations

Code	*Version*	*Organization*	*Country*	*#*	*ID*
MC3d		CEA-ISPN	France	10	MC3DCEA1
IVA	4	Siemens	Germany	7	IVAFZK
	KA	FZK	Germany	8	VA4SIE1
COMETA	1D	JRC	EU	2	COMJRC1D
	2D	JRC	EU	3	COMJRC2D
	IKEJET	Stuttgart University	Germany	1	COMIKE1
IFCI	6.0a	ENEA	Italy	4	IFCENEA1
	6.0a	ENEL	Italy	5	IFCENEL1
	6.01	KAERI	Korea	6	IFCKAER1
JASMINE	2.01	JAERI	Japan	9	JASMJAE1
TEXAS	II	KEMA	Netherlands	12	TEXKEMA1
	IV	Wisconsin University	USA	13	TEXUWIS1
	IV	JRC	JRC	11	TEXJRC1
THIRMAL		SKI/ANL	Sweden/USA	14	THIRANL1
VAPEX		EREC	Russia	15	VAPEX1

Code predicted results are generally affected by quantitative and qualitative uncertainties, which may depend, among others, on modeling and numerical aspects, code option input parameters as well as user or even computer effects. In reactor safety analysis, there is an emerging need to quantify insofar possible or practical the uncertainties associated with code evaluation of accidents and transients in order to provide the basis for a proper evaluation of safety margins and for the adoption of 'best-estimate' rather than restrictive 'conservative' assumptions.

The development/assessment of reactor safety codes is mainly based on experimental data acquired in scaled test facilities since prototypical data from reactor plants are not available for obvious safety reasons inherent to the simulation of accident and transients in nuclear installations. Code application to the full size reactor systems would thus imply the extrapolation of the predictive capabilities accrued in experimental installations which may suffer from scaling distortions and lack of nuclear feedback simulation.

A methodology for the quantification of code uncertainties has been developed at the Department of Mechanical and Nuclear Construction (DCMN) of the University of Pisa; it is based on the Fast Fourier Transform (FFT) technique, which represents code discrepancy in the frequency domain. The FFT methodology is part of the general Uncertainty Methodology and Accuracy Extrapolation (UMAE) approach for the evaluation of uncertainties in predicting accident and transients in nuclear power plants through the extrapolation of accuracy data obtained in scaled test facilities.

2 THE FARO TEST L-14 AND THE ISP-39

2.1 The FARO Test Facility

The FARO test facility became operational in 1987; initially, it was dedicated to the investigation of liquid metal fast breeder reactor severe accident phenomenologies such as melt relocation and molten fuel sodium interaction [2]. On the basis of contingent reactor safety research requirements, the test facility was then reconfigured in the early '90s for the investigation of fuel coolant interaction and quenching phenomenologies pertinent to the progression of severe accidents in water cooled reactors [3]. In its present configuration the FARO test facility consists of 5 main major components which include the furnace, the intersection valve unit, the release vessel, the interaction test section TERMOS and the venting system which are properly instrumented to characterize the evolution of the interaction processes.

2.2 The FARO Test L-14

The ISP-39 reference test case is FARO test L-14 [4] and [5]. It consists of a non-energetic fuel coolant interaction and quenching test in which 125 kg of a dioxide mixture (80%wUO_2 + 20%w ZrO_2) was released by gravity in a 2.05 m deep pool of saturated water at a system pressure of 51 bar. Experimental conditions and results are summarized in Tables 2 and 3, respectively.

The major research objectives assigned to test L-14 included the characterization of the fuel coolant interaction and quenching process under the relevant experimental conditions with emphasis on pre-mixing aspects, debris formation and cooling as well as thermal response of the debris catcher bottom plate. More specific objectives included the evaluation of melt quenching rate and steam production rate, debris particle size distribution, fraction and relocation of unfragmented melt as well as qualitative information on and, as appropriate, quantitative evaluation of hydrogen generation rate.

This initial phase covers the time span from melt release (0 s) up to melt/water contact (0.46 s). The characterizing features of this phase are a small pressure increase (1 bar) resulting essentially from heating of the steam/argon mixture (77w% steam and 23w% argon) in the free-board region and a melt leading edge downward progression at an average rate of 2.04 m/s. There are no direct information on melt jet behavior and break up during this phase; thermocouple measurements indicate, however, that a melt jet leading edge diameter less than 0.3 m is to be postulated at the time of melt/water contact.

Following penetration of the melt into the water pool at 0.46 s, the melt jet progressed downward at an average speed of 5 m/s as inferred from the water pool temperature responses. The melt jet contacted the debris catcher bottom plate at 0.9 s and according to an estimate of the melt trailing edge velocity (2.7 m/s), most of the melt had eventually relocated on the debris catcher bottom plate at 1.62 s.

Steam generation sustained by finer fragmentation and augmentation of heat transfer led to a considerable level swell (1.1 m at time 2.1 s) and to a sharp increase of the pressure (78 bar at 2.4 s) in the TERMOS test vessel. In the long-term phase, the TERMOS vessel pressure increased at a moderate rate as the relocated melt continued to exchange heat with the surrounding medium. After test execution, 124.5 kg of melt were recovered from the debris catcher bottom plate (20 kg as a conglomerate and 104.5 kg as fragments) and 0.5 kg were found on the inner structure of the test vessel. In addition, 31.5 kg of melt, which did not take part in the interaction process, were recovered in form of crust (11 kg on the bottom plate and 20.5 kg in the release vessel).

2.3 ISP-39 Calculation Procedures and Results

ISP-39 was conducted as an 'open' exercise; i.e., in addition to initial and boundary conditions, also the experimental results of the reference test case were provided to the participants at the outset of the exercise. The removal of the classical 'blind' constraints usually attached to an ISP exercise was motivated by the need to decouple to the practical extent code modeling aspects from experimental and measurement uncertainties inherent to the extreme severe accident test conditions.

The participants agreed on the need to adopt, in addition to the specified initial and boundary conditions, a common set of code input parameters in order to have a comparable framework for the conduction of the exercise [6].

The participants were asked to provide a mandatory calculation on the basis of the agreed set of initial and boundary conditions, which is referred to as the reference calculation for the exercise. It was also agreed that additional sensitivity calculations introducing only one parametric variation with respect to the reference calculation should have been considered for an extended comparative analysis.

3 THE ACCURACY QUANTIFICATION METHOD

3.1 Description of the method

The accuracy quantification of a code calculation is based on the amplitude of the FFT of the experimental signal and of the difference between this one and the calculated trend. In particular, the method characterizes each calculation through two values:

– a dimensionless average amplitude

$$AA = \frac{\sum_{n=0}^{2^m} \left| \Delta \tilde{F}(f_n) \right|}{\sum_{n=0}^{2^m} \left| \tilde{F}_{exp}(f_n) \right|}$$

– a weighted frequency

$$WF = \frac{\sum_{n=0}^{2^m} \left| \Delta \tilde{F}(f_n) \right| \cdot f_n}{\sum_{n=0}^{2^m} \left| \Delta \tilde{F}(f_n) \right|}$$

The most significant information is given by AA, which represents the relative magnitude of discrepancy deriving from the comparison between the addressed calculation and the corresponding experimental trend. The WF factor emphasises whether the error has more relevance at low or high frequencies, and depending on transient, high frequency errors can be less important than low frequency ones (in other words, analysing thermalhydraulic transients, better accuracy is generally represented by low AA values at high WF values.

Provided the availability of experimental and calculated trends of the parameter to be analysed, the application of the FFT method implies the following steps:

- selection of analysis time window;
- determination of the number of points;
- determination of the cut frequency value;
- selection of the set of weights.

The choice of the time windows is mainly related to the qualitative accuracy evaluation, and focuses on the identification of the various transient phases, to allow more realistic comparison of involved physical

phenomena and corresponding code models. Since the FFT algorithm requires that functions are identified by a number of values, equally spaced, which is a power of 2, an interpolation generally is necessary to satisfy this requirement. Supposing that available data are characterized by an adequate sampling frequency, the fulfillment of the Sampling Theorem is required to avoid distortion of sampled signals.

All the fifteen calculations submitted to the ISP 39 have been considered for the quantification of the accuracy; the activity has been conducted in the following way:

a) A qualitative accuracy evaluation has been made including engineering (subjective) judgment in the selection of suitable parameters and in the identification of un-suitable calculation results;
b) Application of the FFT based method including the comparison between all measured and calculated trends;
c) The step a), including the obtained results, had no impact on the FFT application;
d) The knowledge and the consideration of the importance of the involved physical phenomena has been kept to a minimal and necessary level to minimize the impact of subjective judgment.

4 CONCLUSIONS

The report described the use of the FFT algorithm for the evaluation of the uncertainties in the predictive capabilities of FCI computer codes when applied in the OECD-CSNI International Standard Problem n. 39 on FARO Test L-14.

The qualitative analysis of the results, as generally performed, was fully discussed in the final report of the ISP 39 exercise and figures of merit of one or another calculation were derived, without a type of classification which was not possible.

It was shown that the FFT response, although being a 'cold' analysis of the data, was able to reproduce in a more objective manner the qualitative observations of the comparisons.

The performed study confirmed the capabilities of the FFT based method in ranking generic calculations results. The use of the method is more powerful when more applications are completed addressing the comparison between measured and calculated trends that characterize the same phenomena. This is the case in the system thermal hydraulics area, where acceptability values for current codes calculation results could be fixed. In this sense, the present application to the study of corium-water interaction must be considered as a pilot one.

ACKNOWLEDGMENT

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UNCERTAINTY EVALUATION OF THERMALHYDRAULIC CODE RESULTS UTILISING UMAE

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1 INTRODUCTION

The need of guaranteeing the integrity of fuel rods in nuclear power plants during off normal situations and accidents led to adopting the conservative approach when utilising thermahydraulic codes and therefore to oversizing every safety related device and every structural element in order to reduce as much as possible the residual risk of radioactive contamination. This implies that the cost of a nuclear installation could be reduced without compromising the safety if a good "best estimate" code together with a reliable uncertainty methodology is available.

The evaluation of the accuracy of large thermalhydraulic codes and of the safety margins of light water reactors are among the objectives of international research programs [1]-[2].

UMAE (Uncertainty Methodology based on Accuracy Extrapolation) has been developed at University of Pisa starting from beginning '80: it is based on the extrapolation of the code error when predicting similar transients in integral scaled facilities. The methodology has been applied so far to five cases with three different codes: CATHARE2, RELAP5 and OLGA.

CATHARE2 is a transient analysis code for complex thermalhydraulic systems, developed at CEN Grenoble (F) by CEA, IPSN, EdF and Framatome to analyse transients in PWR [3].

RELAP5 is a transient analysis code for complex thermalhydraulic systems, developed at INEL [4].

OLGA is a code for the analysis of oil pipelines behaviour (essentially oil-water-sand mixture flowrates and pressure distribution along the pipeline) in annular, stratified, bubble and slug flow regimes [5].

In this paper the basis of the methodology are presented, together with some results coming from three of the above mentioned applications.

2 OUTLINE OF UMAE

The basic idea of the methodology [6] is to get uncertainty utilising the accuracy available from a set of calculations concerning similar transients.

Among the hypothesis of the methodology it is to remind that :

1. the code must be widely used and frozen ;
2. a « homogeneous » set of experimental data must be available, concerning differently scaled facilities (ITF) that are representative of the considered plant, and concerning experiments that are similar to the addressed reactor transient.

It should be emphasised that the experimental data base is not a generic one but it must be chosen carefully through an analysis of the phenomena that characterise the addressed reactor transient and the available transients performed in the facilities.

Provided that the hypothesis are fulfilled, a qualified nodalization of the facilities and of the plant must be developed. The use of a common nodalization, in which corresponding parts of the reactor/facility (e.g. downcomer, upper plenum etc.) are modelled with the same elements (e.g. volume, axial etc.) having the same height, where possible, is a way to reduce the so called "user effect" [7].

The results obtained in this way must be analysed qualitatively and quantitatively, to prevent the user from utilising non-qualified data base while calculating the accuracy.

The qualitative analysis is based on four subjective judgement marks, that are applied both to the matrix of phenomena and to the list of relevant thermalhydraulic aspects. It essentially derives from a visual observation of the experimental and the predicted trends and the following marks are used for the judgement : Excellent (E), Reasonable (R), Minimal (M) and Unqualified (U). A calculation can be accepted if no Unqualified mark is obtained for any of the considered parameters.

The following step is the quantitative accuracy evaluation. Each code run gives a set of curves related to selected parameters that must be compared to the experimental ones. A tool was developed and qualified in the frame of a co-operation between University of Pisa and IPSN [8] to compare calculated and experimental results. It is based on the Fast Fourier Transform (FFT based method). It allows the comparison between two curves in the frequency domain, therefore even transients with different time duration can be compared, and it gives two output for each selected parameter: the Average error Amplitude AA_i and the Weighted Frequency WF_i (the latter is used at present only for a qualitative comparison between trends).

A calculation is accepted only if the pressurizer pressure Average error Amplitude AA is less than 0.1 and the whole Average Accuracy is less than 0.4. These values come from experience in judging calculation results and were fixed during the development of the methodology: they do not depend on the analysed transient or on the user.

Once developed the reactor nodalization, a « Kv scaled » calculation (that is performed with the same boundary and initial conditions as in the tests previously utilised, opportunely scaled) must be done to prove that no new phenomena occur and that the same Relevant Thermalhydraulic Aspects are characterising the results.

The accuracy extrapolation, assuming that the errors are randomly dispersed around the true value of a given parameter, is done utilising the data outcoming from the test calculation. This gives an uncertainty that is used to get the upper and lower envelope of the nominal reactor calculation. It means that for each important point (instant of dryout, PCT, instant of minimum coolant mass inventory etc.) the uncertainty is the average of the errors committed by the code in each of the test calculation for the corresponding variable, plus 2σ (coming from the Gaussian distribution of errors), plus a bias due to the effect of scaling of the facilities considered in the study.

3 UMS APPLICATIONS

UMS (Uncertainty Method Study) was organised by OECD/CSNI to compare the available uncertainty methodologies by applying them to a common exercise. It was chosen to get as "reference nuclear plant" the LSTF facility (the largest PWR simulator available in the world) and as reference transient the Small Break LOCA SB-CL-18, already chosen as International Standard Problem N. 26. The aim of this study was the comparison step by step of the existing methodologies and the comparison of the results with the experimental data [9].

UMAE participated in UMS with two codes, CATHARE2 and RELAP5. The data base for the CATHARE application is constituted by five tests ("counterpart tests") performed in LOBI, SPES and BETHSY, while the one for the RELAP5 application is constituted by ten experiments, including the five "counterpart tests".

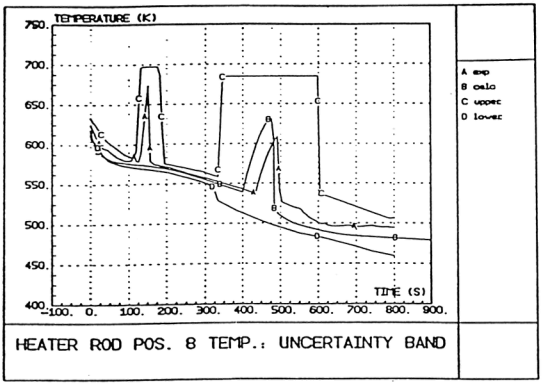

Figure 1: UMS CATHARE application : LSTF heater rod temperature (hot rod, pos. 8), nominal calculation result, uncertainty band and experimental trend

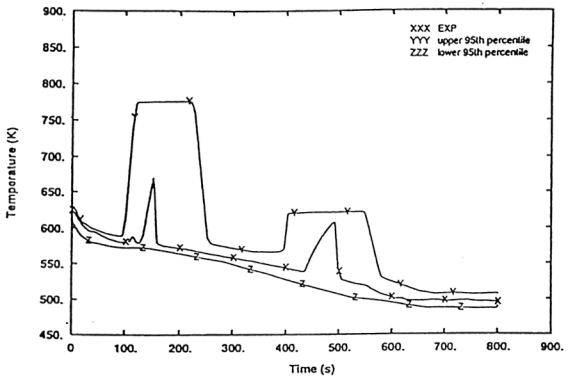

Figure 2: UMS RELAP application : LSTF heater rod temperature (hot rod, pos. 8), nominal calculation result, uncertainty band and experimental trend

The results of the UMS participation of UMAE are presented in Figs. 1 and 2, for CATHARE and RELAP, respectively, in which the uncertainty bands for rod clad temperature are reported. It is to be noticed that the bands bound the experimental data all over the transient and that the resulting PCT is far below the licensing limit (1477 K). Concerning the CATHARE application, in Table 1 some important results are reported.

4 PWR APPLICATION

UMAE was applied to derive the uncertainty relative to a Small Break LOCA in a French NPP [10]. The data base is constituted by the five above mentioned tests and the counterpart test performed in LSTF facility (that was not used in the UMS application as LSTF was the "reference plant"). The initial and boundary condition for the calculation were those relative to normal plant operation.

The result of the uncertainty analysis for the rod clad temperature are presented in Fig. 3. Again it is to be noticed that the PCT is far below the licensing limit.

5 CONCLUSIONS

UMAE (Uncertainty Methodology based on Accuracy Extrapolation) has been applied to derive uncertainty concerning code calculations of PWR and oil pipelines transients with CATHARE2, RELAP5 and OLGA codes.

The results showed in this paper, concerning PWR SBLOCA scenarios analysed with CATHARE and RELAP, demonstrate the applicability of an uncertainty methodology coupled with a Best Estimate code for safety evaluation purposes instead of the conservative approach. This allows to conclude also that the development of a new generation code is no more attractive if there is available a reliable uncertainty methodology that overcomes actual Best Estimate code limitation.

SIMBOLS AND ABBREVIATIONS

CEA	Commissariat a l'Energie Atomique
EdF	Electricité de France
FFT	Fast Fourier Transform
INEL	Idaho National Engineering Laboratory
IPSN	Institut de Protection et Sureté Nucléaire
ITF	Integral Test Facility
LOCA	Loss of Coolant Accident
NPP	Nuclear Power Plant
PCT	Peak Clad Temperature
UMAE	Uncertainty Methodology Based on Accuracy Extrapolation
UMS	Uncertainty Method Study

Table 1: Relevant point quantities concerning the UMS CATHARE application

Quantity	Range	Notes
First peak clad temperature (PCT1)	573+120K −20K (**)	
Second peak clad temperature (PCT2)	631+50K − 120K (**)	
Time of first peak clad temperature	165 ± 30 s	
Time of second peak clad temperature	476 ± 154 s	
Time of overall peak clad temperature	476 ± 154 s	
Minimum core pressure difference	Not calculated	It is possible to calculate such a quantity

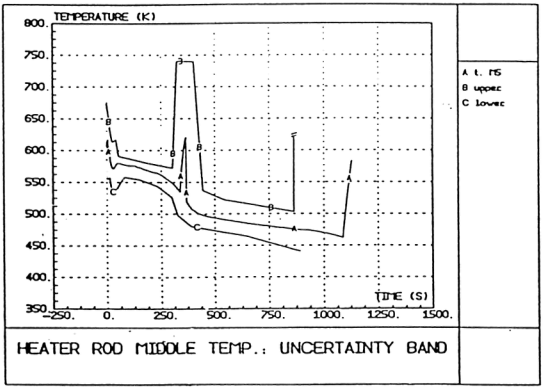

Figure 3: CATHARE application - PWR fuel rod temperature, nominal calculation result and uncertainty band

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SYSTEMS-LEVEL SENSITIVITY ANALYSIS, RESPONSE SURFACE COMPARISONS, AND DIAGNOSTIC TESTING FOR EVALUATION OF EULERIAN AIR QUALITY MODELS

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1 INTRODUCTION

Air quality models (AQMs) are widely used to assist environmental decision-making by predicting the future emissions reductions which would be required to meet mandated air quality goals. Given the very large economic and social costs of decisions affecting ozone (O3) control we wish to avoid potential mistakes by using the AQMs to provide a realistic simulation of future conditions and an accurate appraisal of the type and amount of emissions reductions necessary to meet the air quality goals. Thus, evaluating the sensitivity of air quality predictions to estimated changes in emissions is a significant part of confirming these physically-based models. For complex models, we cannot understand this sensitivity to changes and uncertainties unless we understand the details of the dynamic interactions among competing processes.

The air quality system, particularly as related to O3, is a nonlinear system with major auto-catalytic cycles. The nonlinear production of O3 in the troposphere can be represented as a response surface having two domains separated by a ridgeline of maximum O3 concentration ([O3]) as shown in Figure 1. The ridgeline marks an area of subtle changes in the effectiveness of control strategies for minimizing [O3], depending on whether the region to be controlled is limited by the availability of nitrogen oxides (NOx = NO + NO2) from NOx emissions, or of radicals from emissions of volatile organic compounds (VOC). The response surface is typically depicted through sensitivity analysis with simple models and analytic tools such as the OZIPR and EKMA. The Eulerian 3-dimensional models are generally thought to represent the physical system better than the simple models through their incorporation of complex meteorological processes and other physical phenomena affecting the photochemical production and transport of pollutants. However, for both simple and complex models, the uncertainties in inputs, parameterizations of processes, and incomplete or inaccurate descriptions resulting from ignorance about the physical system produce two areas of uncertainty and potential for error: (1) in the depiction of where a particular photochemical system is in the response space; and (2) in the shape of the response surface. These errors may reduce a model's scientific credibility, and could lead to costly mistakes in guidance for air quality decision-making.

To avoid such errors we must characterize and understand the constituent processes in AQMs and learn how those processes interact to produce model predictions. Furthermore, we should test elements of these model processes, in addition to the model's final predictions, against data from the physical system of the real world to ascertain the fidelity of the model's process representations. Using models instrumented to provide specific details of their process characteristics has taught us that seeing only model resultants -- *e.g.*, time series or final concentrations -- gives an incomplete or distorted picture of the model's behavior since the multiple interactions and feedbacks of the underlying processes that act to produce the resultants are not revealed in those apparently simple answers. For this reason, we cannot depend solely on the typical approaches, including traditional sensitivity analysis on resultants, to evaluate the applicability of these models. By additionally probing the models in a diagnostic way we can illuminate their processes and interactions and can also aid in the interpretation of results from traditional sensitivity analyses with increased accuracy. In this way, systems-level sensitivity analysis supported by process-oriented diagnostic testing allows for better confirmation of the physically-based AQMs, and for greater confidence in using the models in environmental decision-making.

2 METHODS AND RESULTS

There is increasing interest in the AQM community to develop and test meaningful indicators of the photochemical system's sensitivity to changed emissions and meteorology. One set of indicators has been developed around the concept of radical initiation and propagation, and the underlying nonlinear NOx and VOC cycles. We find that

diagnostic testing using such indicators provides unique insight about the fidelity of the physical and chemical processes represented in the model. Two categories of diagnostic tests we have carried out are discussed here: (1) response surface diagnostics dealing with the shape of the O3 response surface and location of a modeled region on it; and (2) process diagnostics designed to probe the model's internal representations of the chemical and physical interactions and feedbacks that ultimately control the production of O3. As an aid to understanding our techniques for sensitivity analysis and process-oriented testing, we begin with a brief overview of the chemistry of O3 formation.

3 NOx-OH PHOTOCHEMISTRY AND THE O3 RESPONSE SURFACE

Ozone production in the troposphere is dependent on the concentrations of reactive forms of NOx, and on the competing interactions and feedbacks of NOx with VOCs. Production of O3 (P(O3)) is initiated by photolysis of background O3 and formaldehyde to create hydroxyl radical (OH). This initiation is followed by propagation of the radical by means of OH attack on carbon monoxide (CO) and VOCs to produce the peroxy radicals HO2 and RO2. Peroxy radicals then react with available NO to produce NO2, and recreate some fraction of the original OH. Thus, we define the efficiency with which OH is propagated, Pr(OH), as the average number of OH radicals recreated for each initial OH; in a related way, we define the OH chain length as the average number of times one OH cycles through the system, which can be calculated as 1 / (1- Pr(OH)). However, the OH propagation will be only a fraction of the initial OH due to the destruction of OH or RO2 and HO2 radicals in termination reactions that produce HNO3 (from OH + NO2) and peroxides (from peroxy self-reactions).

While the photolysis of NO2 to give NO and excited monatomic oxygen (O3P) begins the process of forming O3 from O2, due to the rapid back reaction of O3 with NO, P(O3) by this pathway would cease without the competitive OH propagation reaction pathway to oxidize NO to NO2. The result of these interrelated events and reaction cycles is that several O3 molecules can be created before NOx terminates and is removed from the system. Hence it is the change in competition among the reactions of the OH and NOx cycles brought about by different levels of NOx and VOC that produces the O3 response surface shown in Figure 1.

Figure 1 shows the response surface for maximum [O3] from a simulation for Atlanta, GA. The contour lines of the surface are derived by fitting contours to the peak model-predicted [O3] in multiple simulations using different VOC and NOx emissions. The heavy line cutting across the surface contour lines and dividing the response surface into two domains is the ridgeline of maximum [O3], and corresponds to the region of maximum Pr(OH) and the greatest OH chain length.

Production of O3 in the domain above the ridgeline is limited by the availability of radicals. Under conditions of high [NOx] in this radical-limited domain, NO2 reacts with OH and terminates to HNO3, thereby removing both an OH and an NO2 which limits P(O3) by reducing Pr(OH). Furthermore, NO titrates O3 and reduces this source of initial OH. In these cases, the efficiency of O3 production per NOx terminated is low, and P(O3) is more responsive to reductions in VOCs than in NOx.

In systems with low [NOx], NO is relatively less available, allowing the peroxy radicals RO2 and HO2 to self-terminate and reduce the OH chain length and the efficiency of the NO to NO2 conversion per radical. Termination of

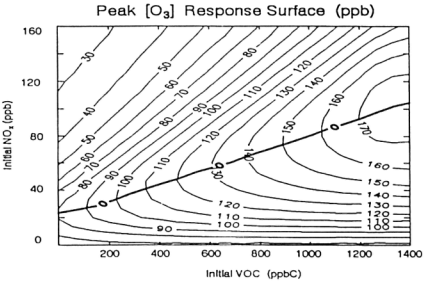

Figure 1

NO2 by OH is also reduced due to decreased available NO2. Hence in these cases, although the efficiency of P(O3) per NOx terminated is high, less available NOx results in lower P(O3) and less final O3. Systems in this NOx-limited domain below the [O3] ridgeline are thus more responsive to reductions in NOx than in VOCs.

4 PROCESS-ORIENTED DIAGNOSTICS FOR INDICATORS OF O3 SENSITIVITY

In this section we provide brief descriptions of some sensitivity indicators and diagnostic probes of model processes, and present results of preliminary applications in several model simulations.

Case 1. Meteorology and Emissions Uncertainty. Uncertainties in some key elements of the emissions and meteorology for AQMs are in the range of 50% to 100%, with some areas of emissions uncertainty even higher. Sensitivity analyses have been used to characterize the effects of these uncertainties in peak predicted [O3]. However, a central question remains: "How do the uncertainties affect the control strategy predictions of the AQMs?" These are the predictions of the relative changes in O3 due to changes in emissions, and predictions of a preference for NOx or VOC controls. A full, brute-force sensitivity analysis of the effects of mixing height uncertainty on the sensitivity of the daytime O3 response to a 15% reduction in NOx emissions shows there is a systematic shift in the O3 response (expressed as a per cent change from the base case), regardless of the meteorology conditions and hence daytime [O3]. See Figure 2.

The per cent change in [O3] due to a 15% reduction in NOx emissions is shifted several percentage points higher when the mixing height is reduced. This means that the system is systematically moving on the O3 response surface towards the radical-limited domain, and hence changing the relative effectiveness of NOx and VOC controls. As shown in Figure 3, the change in daytime [O3] due to the change in mixing height is small for 9 out of the 25 days simulated, and is not well-correlated with the shift in control strategy effectiveness.

From the theoretical perspective we described just above where P(O3) is driven by the product of radical initiation and OH chain length, we have developed indicators of the position of the system relative to the [O3] ridgeline. One such robust indicator is [O3]/ NOx]. Figure 4 shows that the per cent change in [O3]/ NOx] due to the change in mixing height is strongly predictive of the resulting change in control strategy effectiveness; *i.e.*, the change in the indicator tracks the system change on the response surface. The change in the resultant, [O3], on the other hand, does not provide insight into how the system sensitivity is being changed.

Case 2: OH + NO2 Rate Change. Experiments were run to test the effects of a change in the rate constant for the reaction of OH with NO2 to produce HNO3, one of the most sensitive reactions in the chemistry and crucial for the propagation of OH and P(O3). We evaluated whether adopting a proposed new rate ~20% lower than the one currently used in most AQMs would have significant effects on [O3], and whether indicators of the internal changes in model processes could be used to understand those effects. Because changing the OH + NO2 reaction rate changes the availability of OH and NO2, we also expected to see effects of such a change in the relative sensitivity of P(O3) to changes in NOx and VOC emissions (Emis_NOx; Emis_VOC).

Using OZIPR and EKMA we simulated conditions for Atlanta, GA in a base case and for the same case with the OH + NO2 rate 20% lower. Looking only at the percent change in peak [O3] from the base case to the altered one, we saw

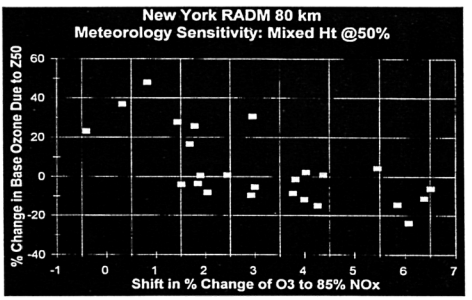

Figure 2

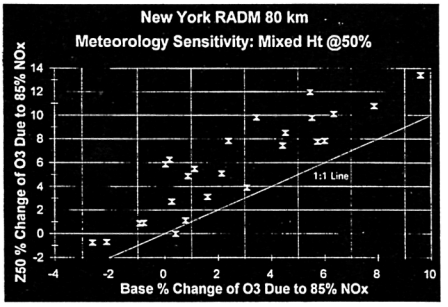

Figure 3

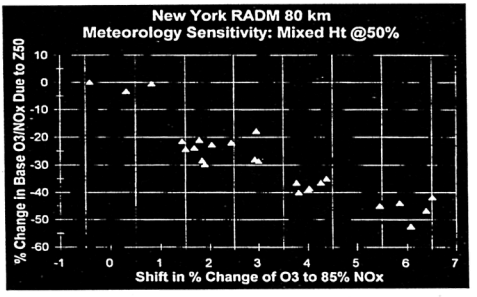

Figure 4

a small increase of ~2% in peak [O3] for conditions where [NOx] was less-than 20 ppb, a ~6% increase for conditions near the [O3] ridgeline, and still larger increases as the system moves over the ridge into the radical-limited domain that characterizes some urban core systems. The changes in average [OH] with increasing [NOx] track this change in [O3].

Diagnostic probing of the process changes in the photochemistry allowed us to account for these changes -- which were surprisingly small given the central role of the OH + NO2 reaction -- as direct and indirect effects in the OH-NOx chemistry. The direct effect of lowering this reaction rate is to increase available OH and to increase the fraction of OH attacking VOCs. For the case we simulated, this effect accounts for ~30% of the change in [O3]. The indirect effects of changed radical propagation efficiency and increased OH chain length account for the rest of the increase.

Changing the OH + NO2 rate also changed the sensitivity of [O3] to changes in VOC or NOx emissions (d[O3]/d[Emis_VOC] or d[O3]/d[Emis_NOx]). These sensitivity results differ for systems that are either VOC-limited or NOx-limited. For example, d[O3]/d[Emis_VOC] in strongly radical-limited systems is increased by 20% to 40% compared to simulations with the base case reaction rate, and is decreased slightly in NOx-limited systems. This has the effect that VOC controls modeled using the new reaction rate become more effective for the radical-limited systems, and slightly less-effective for the NOx-limited ones relative to the controls calculated using the old reaction rate. Taking into account the more complicated changes in d[O3]/d[Emis_NOx], VOC controls are made slightly less-effective relative to NOx controls using the new lower reaction rate. However, target levels of [O3] are made more difficult to reach because the lower rate actually increases the efficiency of P(O3) per NOx, and the peak [O3].

5 SUMMARY

To understand a complex model's predictions of resultants and their sensitivity to changes and uncertainty we must probe and understand the model's underlying processes and cycles and their competing interactions. In our initial testing in the radical-limited domain of the [O3] response surface, our techniques and the interpretations of model behavior made possible with indicators based on combinations of resultant species have provided useful information about the model's processes and its sensitivity to change. Work to develop and test other indicators that evaluate systems-level sensitivity and process-level dynamics continues in our research group.

There is now strong evidence emerging that the AQMs are getting the right resultant [O3] for the wrong reasons; *i.e.*, that the resultants are produced through the interaction of compensating errors in model processes. This means that the [O3] response surface is in error, and hence that model predictions of O3 sensitivity to changed emissions used in air quality decision-making will have an unknown bias. Given the necessity of having a process-level understanding of the models, traditional sensitivity analysis on resultants is inadequate to properly characterize that bias and point to possible errors in the models' physics and chemistry. Thus, to depict and explain the unknown bias, and to improve the models, we require systems-level sensitivity analysis and process-oriented diagnostic testing. These techniques are powerful new evaluation elements for significantly enhancing the testing and confirmation of these physically-based process models.

DETERMINATION OF THE OPTIMAL INPUTS FOR AN IDENTIFICATION PROBLEM USING SENSITIVITY ANALYSIS

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1 INTRODUCTION

System identification may be defined as the process of determining a model of a dynamical system using observed input and output data. In the event that the model is given and only its parameters are unknown, system identification reduces to parameter estimation.

Due to importance and necessity of accurate parameter determination, many methods for linear and nonlinear system parameter identification have been developed (see, for example [1], [4]). Observed data for parameter estimation are often both difficult and expensive to obtain. Thus, in performing an actual experiment, it is desired to obtain the maximum benefit from the observations. In particular, the input to the system should be such that it maximizes the sensitivity of the state variable to the parameter ([2], [3], [4]).

In the last decade the role played by the sensitivity functions in the theory of optimal design became much better understood. It is well known that the absence of smoothness or continuity for the sensitivity functions associated with a system is closely connected with discontinuities in the state of the system, with lack of smooth properties of design vector, and possibly with bifurcation phenomena ([5]).

The object of this paper is to analyze numerically a sensitivity criterion associated with a parameter identification problem corresponding to an elliptic partial differential equation.

Specifically, we treat with the maximization of the sensitivity of the parameter-to-solution mapping for the model equation

$$\begin{cases} -\Delta u + qu = f, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega. \end{cases} \tag{1}$$

That is, the input function f is chosen such that the sensitivity of the solution $u(q)$ of (1) with respect to the parameter $q \in Q_{ad}$ (the set of admisible parameters) is maximized. Following the theoretical setup in [3] we use an appropriate measure for the sensitivity of determining $q \in Q_{ad}$ from the solution $u(q)$ of (1).

The above inverse problem (estimation of the parameter $q(x)$ from the available data for u) is of great interest and has been extensively studied as a model problem for parameter estimation in elliptic partial differential equations. Finding the optimal location or distribution of the source function f that maximizes the recovery of q from measurements of $u(q)$ is a problem of practical importance. The sensitivity measure will be constructed through the linearization of the solution map $q \in Q_{ad} \to u(q)$ at a reference point $\overline{q} \in Q_{ad}$. In terms of the inverse problem, $\overline{q}$ is chosen as the best *a priori* guess to the unknown parameter.

2 THE FUNCTIONAL FRAMEWORK

We briefly describe the theoretical framework applied to the specific example in Section 3. Let G_f be a family of nonlinear mappings from a subset of a Hilbert space X into a Hilbert space Y. We are concerned with the selection of an optimal f such that the inversion of G_f becomes as stable as possible. The mapping $q \to G_f(q)$ can typically arise as the solution mapping for a partial differential equation, with q representing a coefficient or an inhomogeneity of the differential equation. The functional parameter f represents a *design* parameter which is selected from a class of admissible input functions $\mathcal{F}$. The

problem of optimal experimental design can be formulated as follows: Choose the best input f for the reconstruction of the coefficient q from knowledge of $G_f(q)$, the state of the differential equation.

For the selection of the optimal parameter f we proceed as follows. Let $G'_f(q)$ be the linearization of G_f at some reference point $q \in X$, and consider

$$\sup_{f\in\mathcal{F}} \inf_{\substack{h\in V\\ h\neq 0}} \frac{|G'_f(q)h|_Y^2}{|h|_X^2} \tag{2}$$

where $V \subset X$ is a Hilbert space continuously embedded in X. Thus, from (2) we notice that we propose to maximize the lowest singular value of $G'_f(q)$ (considered as unbounded operator between X and Y) as f varies in $\mathcal{F}$.

Turning to the infimum problem

$$\inf_{\substack{h\in V\\ h\neq 0}} \frac{|G'_f(q)h|_Y^2}{|h|_X^2} \tag{3}$$

in (2) we notice that the mappings G_f are illposed in the sense of lack of continuous invertibility. For (3) to be nonzero an estimate of the type

$$|G'_f(q)h|_Y \geq \kappa_f |h|_X\,, \qquad \text{for all} \quad q \in V. \tag{4}$$

is necessary with κ_f a positive constant, possibly depending on $f \in \mathcal{F}$.

3 SPECIFIC EXAMPLE

We put $\Omega = (0,1)$ and consider the following elliptic equation:

$$\begin{cases} -\Delta u + qu = f, & \text{in} \quad (0,1), \\ u(0) = u(1) = 0, \end{cases} \tag{5}$$

for the determination of the function $q(x)$ from data for u.

For $q \in Q_{ad} := \{q \in L^\infty(0,1) : 0 < q_m \leq q(x) \leq q_M \text{ a.e. on } (0,1)\}$, we define $A(q) : H^2(0,1) \cap H_0^1(0,1) \to L^2(0,1)$ by $A(q)u = -\Delta u + qu$. One can argue that the solution map $u : Q_{ad} \subset Q = L^\infty(0,1) \to H^2(0,1)$ is continuously Fréchet differentiable and the Fréchet derivative at q in direction $h \in L^2(0,1)$ is given by $v = u'(q)h = -A^{-1}(q)(hu(q))$.

We choose $\varepsilon \in (0,1)$ and consider the class of admissible input functions $\mathcal{F} = [\varepsilon, 1-\varepsilon]$. For $\alpha \in \mathcal{F}$ we define

$$\eta_\alpha(x) = \begin{cases} 1 & \text{for} \quad x \in \left[\alpha - \frac{\varepsilon}{2}, \alpha + \frac{\varepsilon}{2}\right], \\ 0 & \text{otherwise.} \end{cases}$$

The inhomogeneities f in (5) are chosen in the class of functions $\{\eta_\alpha : \alpha \in \mathcal{F}\}$. We define the operators $T_{\eta_\alpha} h = -A^{-1}(q)(hu(q;\eta_\alpha))$, for $h \in L^2(0,1)$. Following the theoretical setup in [3] one can show that there exists $K > 0$ such that the bilinear form

$$a_{\eta_\alpha}(h,h) = \langle T_{\eta_\alpha} h, T_{\eta_\alpha} h\rangle_{L^2(0,1)} + \beta\langle h, h\rangle_{L^2(0,1)} \geq K|h|^2_{L^2(0,1)},$$

for all $h \in L^2(0,1)$ and $\alpha \in \mathcal{F}$. The scalar β plays the role of an regularization parameter. The Fréchet differentiability of the eigenvalues and eigenvectors of A_{η_α} (the operator associated to the bilinear form $a_{\eta_\alpha}(h,h)$ by the Lax-Milgram theorem) result from Corollary 2.9 and 2.10 in [3].

Thus, the saddle point problems are given by

$$\sup_{\alpha\in\mathcal{F}} \inf_{\substack{h\in L^2(0,1)\\ h\neq 0}} \frac{a_{\eta_\alpha}(h,h)}{|h|^2_{L^2(0,1)}}. \tag{6}$$

4 NUMERICAL IMPLEMENTATION

All the numerical experiments were performed using Matlab routines (version 4.2) running on a personal computer IBM DX4 at 100 Mhz. We performed three numerical tests using both constant parameters (the first test, Figure 1.a–1.c) and functional parameters (the other two tests, Figure 1.d–1.i) with the following input data: $N = \dim H^N = 16$, $\varepsilon = 0.5$, $\beta = 10^{-5}$. We used the Matlab function ***eig*** to solve the generalized eigenvalue problem (8).

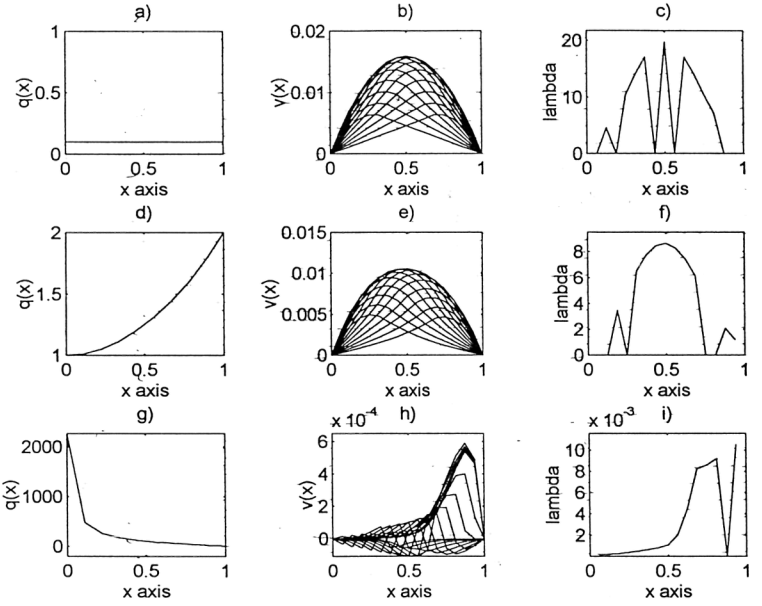

Figure 1: The plots representing the parameter q (left side, subplots 1.a,1.d and 1.g), the first eigenvalue λ (right side, subplots 1.c, 1.f and 1.i) and the sensitivity functions v (middle position, subplots 1.b, 1.e and 1.h).

For the discretization we choose subspaces

$$H^N = \{h^N = \sum_{i=1}^{N/2} h_i B_i^N, \quad N \text{ even}\},$$

and B_i^N are piecewise constant functions with value 1 on $\left[\frac{2(i-1)}{N}, \frac{2i}{N}\right]$ and value 0 outside this interval. For given $\alpha \in \mathcal{F}$ and $q > 0$, the approximate solution $u^N(q, \eta_\alpha)$ to (5) was determined as the Galerkin

solution with respect to the discretization of (5) by linear spline functions on the grid $\{\frac{i}{N}\}_{i=0}^{N}$. The approximate minimization problems are then given by

$$\min_{\substack{h^N \in H^N \\ h^N \neq 0}} \frac{a_{\eta_\alpha}^N(h^N, h^N)}{|h^N|^2_{L^2(0,1)}} \tag{7}$$

where $q_{\eta_\alpha}^N$ is defined like q_{η_α} with $u(q, \eta_\alpha)$ replaced by $u^N(q, \eta_\alpha)$. The solution to (7) is characterized by the smallest eigenvalue of the generalized eigenvalue problem

$$A_{\eta_\alpha}^N \vec{h}^N = B^N \vec{h}^N \tag{8}$$

and the minimum in (7) is assumed at the eigenfunction associated with the smallest eigenvalue. In (8), $\vec{h}^N$ denotes the coordinate vector of h^N, and $A_{\eta_\alpha}^N$, B^N are the matrix representations of the forms $a_{\eta_\alpha}^N(h^N, h^N)$ and $\langle h^N, h^N \rangle$ on $H^N \times H^N$, respectively.

If we suppose that the process governed by the model equation (1) is observed in a single point x_0 in the domain Ω we can determine the optimal location of this point in order to have the sensitivity function maximized. The profiles of the sensitivity functions v corresponding to the parameter q is illustrated in Figure 1 (subplots 1.b, 1.e, 1.h). The observation point x_0 is taken arbitrary in the space interval $[0, 1]$. For the case when the parameter q is constant ($q = 0.1$, subplot 1.a) and in the case when $q(x) = 1 + x^2$ (subplot 1.d) the sensitivity function v attains a maximum value near the middle of the interval $[0, 1]$. In the last example we have chosen a parameter with large amplitude in the space interval $[0, 1]$ in comparison with the previous examples. In this case we put $q(x) = 1.5 + 100|\tan^{-1}(1500(x - .4))|$. The sensitivity function gradually increases in the interval $(0, 0.75)$ attains a maximum value in the interval $(0.75, 0.9)$ and then decreases abruptly to the end of the interval $[0, 1]$ (subplot 1.h). Hence, in the identification problem associated with (1) is not recommended to place observation points outside the interval $(0.75, 0.9)$ where the system presents a low sensitivity. Otherwise, one would obtain relatively "bad" estimations of the parameter to be identified.

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THE BAYESIAN APPROACH TO MODEL UNCERTAINTY: METHODS AND APPLICATIONS

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Stochastic models are central to scientific inference and decision-oriented prediction in many fields. Such models typically are based on a single set of *structural assumptions* about how outcomes of main interest are related to relevant predictor variables. Some aspects of these structural assumptions are specified by the theory underlying the attempt at inference or prediction, but theory rarely fully specifies structure; instead a number of structural details are typically chosen with the aid of the available data. The resulting stochastic model will usually contain *parameters* (unknown constants) whose meaning is particular to the chosen structure. It is routine, in using such models to draw inferences about those parameters and make predictions, to acknowledge *parametric uncertainty* conditional on the chosen structural form, but it is considerably less common to acknowledge the *structural uncertainty* implied by the data-driven search to fully specify the model in the first place. The result can be uncertainty assessments that considerably overstate inferential and predictive accuracy, leading to inaccurate scientific summaries, overconfident decisions, and flawed risk assessments.

To see how to improve on usual practice in this respect, it is useful to observe that in many basic problems of inference and prediction in science and decision-making (see, e.g. [1,2]), six ingredients are recognizable:

- Past data D, both observable in principle and actually observed.
- One or more quantities of interest Q, which may include future observable data and/or inherently unobservable quantities.
- Model *scenario* input(s) X. A scenario is a description that characterizes the likely values for the predictor variables serving as inputs in the modeling process, for example at a given time in the future under a particular public policy.
- Model *structure* S. This refers to modeling ingredients such as (a) the functional form by which the outcome variable $Y = f(X)$ is taken to depend on the predictor(s) X, apart from unexplained variation, and (b) the choice of which of the available X_j should be employed in the modeling and which can be ignored.
- Model *parameters* θ_S, conditional on scenario and structure. A particular structure S typically specifies not just a single model but an entire family of models, indexed by one or more parameters. For any given structure S there is typically little ambiguity about the set Θ_S of *possible* parameter values corresponding to S, but the relative *plausibility* of each value of θ in Θ_S requires assessment in light of the data D.
- Model *predictive* uncertainty, conditional on scenario, structure, and parameters. This ingredient is needed because even if the three previous ingredients were "known perfectly," the model predictions may still differ from observed outcomes (due, e.g., to measurement inaccuracies and to not having considered all possible scenarios and structures).

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With this formulation of the problem, the goal is an uncertainty assessment about Q in light of D that properly accounts for scenario, structural, parametric, and predictive uncertainty about the model, M (say). It is routine in the classical—frequentist—statistics paradigm, widely employed in science and decision-making, to assess parametric and predictive uncertainty and propagate these two through to your final inferential and predictive answers, but it is much less common in practice to fully account for scenario and (especially) structural uncertainty, mainly because the latter form of uncertainty is hard to conceptualize in the frequentist approach to probability [3].

In recent years a nonclassical, Bayesian approach to this problem has been gaining acceptance in statistical theory and applications [1,4]. With this approach all sources of uncertainty may be quantified by means of conditional probability distributions, and the basic principle governing the calculations is that *you should condition on things that you are certain about and average over your uncertainty about things that you're not certain about*. The key equation making this principle operational in this situation is

$$p(Q|D,\mathcal{M}) = \int_{\mathcal{M}} p(Q|D,M)\, p(M|D)\, dM, \tag{1}$$

where $\mathcal{M}$ is the class of models capturing all relevant scenario and structural choices and their corresponding parametric and predictive possibilities. In words, equation (1) says that your conditional distribution for Q, given D and based on the choice of model class $\mathcal{M}$, is a weighted average of the conditional predictive distributions $p(Q|D,M)$ specific to each model M in $\mathcal{M}$, weighted by the relative plausibility of the models as measured by their posterior probabilities $p(M|D)$ given the data. Note that equation (2) only makes sense if Q has the same meaning in all models in $\mathcal{M}$; this will be automatically true if Q is a future observable quantity, but when instead Q is an unobservable parameter, care must be taken in specifying $\mathcal{M}$ so that unlike quantities are not mixed together in the weighted average.

In practice equation (1)'s simplicity masks a fair amount of work, since the models $\mathcal{M}$ being averaged (integrated) over have four components: the set $\mathcal{X}$ of scenarios X, the set $\mathcal{S}_{\mathcal{X}}$ of structures S_X, the set Θ_S of possible values for the parameters θ_S, and the predictive distributions $p(Q|D,M)$ themselves. In the fullest generality equation (1) thus requires three levels of integration:

$$p(Q|D,\mathcal{X},\mathcal{S}_{\mathcal{X}}) = \int_{\mathcal{X}}\int_{\mathcal{S}_{\mathcal{X}}}\int_{\Theta_S} p(Q|X,S_X,\theta_S)\, p(\theta_S|D,S_X)\, p(S_X|D,X)\, p(X|D) d\theta_S\, dS_X\, dX. \tag{2}$$

Here $p(Q|X,S_X,\theta_S)$ is the conditional distribution for Q given specific choices for scenario, structure, and parameters, and $p(\theta_S|D,S_X)$, $p(S_X|D,X)$, and $p(X|D)$ are the *posterior distributions* for the parameters, structure, and scenario (respectively) given the past data.

Each of these posterior distributions in turn depends on *prior distributions* specifying what, if anything, is known before the data D arrive. For example, the posterior $p(S_X|D,X)$ for structure given the data and a particular scenario X is a multiplicative function of the prior $p(S_X|X)$ on structure and the *likelihood* $p(D|S_X,X)$ for the data given structure,

$$p(S_X|D,X) = c\, p(S_X|X)\, p(D|S_X,X), \tag{3}$$

where c is a normalizing constant.

In some cases scenario-specific solutions are required, rather than an answer that propagates scenario uncertainty. Equation (1) is simpler in this situation:

$$p(Q|D,X,S_X) = \int_{S_X}\int_{\Theta_S} p(Q|X,S_X,\theta_S)\, p(\theta_S|D,S_X)\, p(S_X|D,X)\, d\theta_S\, dS_X. \tag{4}$$

Application of equations (2) and (4) presents two types of challenges, one technical and the other substantive.

- *Technical challenge:* Computing with the formulas above requires the evaluation of difficult, often high-dimensional integrals, e.g., the likelihood $p(D|S_X,X)$ in equation (3) above is of the form

$$p(D|S_X,X) = \int_{\Theta} p(D|\theta_S,S_X,X)\, p(\theta_S|S_X)\, d\theta_S, \tag{5}$$

  and the parameter vector θ_S given a particular structure S_X may well be of length greater than (say) 50. The leading current technologies for overcoming this challenge are *Laplace approximations* (e.g. [5]) and *Markov Chain Monte-Carlo integration* [6].

- *Substantive challenges:*
  - Q: How can you be sure that $\mathcal{X}$ contains all relevant scenarios and $\mathcal{S}_{\mathcal{X}}$ contains all plausible structural choices? A: You can't; in practice you just try to be as exhaustive as possible given current understanding and resource limitations. There is no good way in this (or any other) approach to completely hedge against unanticipated combinations of events that have never happened before. It is tempting to set aside a bit of probability for what might be termed the *category "other,"* but how much probability should it have, and where (in model or outcome space) should it be located? For example, if you were trying to forecast oil prices and you were making predictions in 1965 (say), how could you prospectively allocate probabilities and consequences to events like the 1974 Arab oil embargo which had never happened before?
  - Q: Where do the prior distributions $p(X)$ and $p(S_X)$ on scenarios and structures come from? A: One good approach is to start with expert judgment to tentatively specify $p(X)$ and $p(S_X)$, use *sensitivity analysis* [7] to see how much the final answers depend on these priors, and *tune* them using *predictive calibration*: (a) compare observed outcomes to their predictive distributions given past data—if the observed outcomes consistently fall in the tails of these distributions, then the priors may well have been inaccurately specified, so (b) respecify them and go back to (a), iterating until the predictions are well-calibrated. To avoid using the data twice this is best done [8] by dividing the available data D at random into three parts: (i) a part on which the models are fit, (ii) a part on which the iterative calibration of the priors is conducted, and (iii) a part on which the overall machinery developed in (i) and (ii) is itself checked for calibration.

In the paper described by this extended abstract I illustrate the methods described above with a case study (GESAMAC) which involves assessing the risks associated with underground disposal of spent nuclear fuel rods [2]. My partners and I on the GESAMAC project will in this paper present the first results in this field which feature the propagation of uncertainty across a wide variety of scenarios—including (a) a fast pathway to the biosphere, (b) an additional geosphere layer, (c) glacial advance, (d) environmentally induced changes, and (e) human disposal errors.

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CONCEPTUAL UNCERTAINTIES IN SOLUBILITY CALCULATIONS IN GROUNDWATER SYSTEMS: A CALCULATION EXERCISE

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1 INTRODUCTION

Over the last decades, several methods for determining the uncertainties and sensitivities of results from computer simulations, have been developed, e.g. [1, 2, 3]. Some of these techniques have been used for investigations of various problems ranging from economics to the nuclear fuel cycle.
Unfortunately, in many cases the largest uncertainty does not lie in the effect of input parameter uncertainties, but rather in the choice of model to use in the calculations. In this paper solubilities are calculated for some actinides in the presence of uncertainties due to rock-water interactions. The uncertainties induced in such calculations due to uncertainties in thermodynamical data are not included since they have been reported elsewhere [4, 5]. Four different methods to perform solubility calculations have been considered. They all have the common factor that they may be motivated by different experimental ways to mirror reality.

2 METHOD 1, ISOLATED DISSOLUTION

In the first method, the water composition is supposed to be known, measured or calculated, within uncertainty limits and the rock - groundwater interaction during dissolution/precipitation reactions are neglected. This method is analogous to laboratory measurements in which water is sampled from a borehole and then equilibrated it with the desired solid phase. In the case presented here, the water composition was obtained by rock water interaction calculations. The MINVAR program [6] produced mineral sets from mineral abundances and associated uncertainties given by [7] using the Latin Hypercube (LHS) technique. The resulting mineral sets were used as inputs to the CRACKER program [8] which calculated simulated groundwater compositions. From the results a mean water composition and uncertainty intervals for the properties were calulated. Those results were propagated to the UNCCON program where the effect on the calculated solubilities were obtained. Also in this case the LHS technique was used.

3 METHOD 2, ONE MINERAL

This method is similar to the first, with the difference that the dissolution/precipitation reactions are assumed to take place in the presence of one randomly choosen mineral. In old fractures large areas of the fracture walls are covered with only one mineral. If such a fracture ends close to the repository the solubility of any released elements will be determined by the presence of this mineral. And if such a slab is encountered further away it will determine the element concentration along the fracture.

4 METHOD 3, SIMULATED WATER PUMPING

In the third method, the solubility is calculated in the presence of different minerals at different locations across a fracture surface. In this case, the water properties are allowed to vary locally while the water propagates along the fracture. The resulting waters are then mixed to form a simulated sample. During this simulated sampling process, no dissolution/precipitation reactions are supposed to take place.
It is natural to assume that if the water flowing through a fracture is allowed to equilibrate with each mineral grain and the solid phase considered, i.e. $Pu(OH)_4$. The MINVAR program has been used to produce 30 mineral sets which were used by CRACKER to find local solubilities. For each case, 30 equilibrium waters are mixed to form a final solution.

5 METHOD 4, SIMULATED RANDOM SAMPLING

This method is similar to the simulated pumping method except that no pumping is simulated. Instead the full range of solubilities in the fracture are investigated. This method is a complement to method two in the sence that the solubilities are given by one mineral at a time, but the water is allowed to vary to a larger extent. Solubility values are sampled from some 3000 locations along a simulated fracture.

6 RESULTS

The results are mainly statistical estimators such as mean and variance of the solubilities. In addition, for three of the calculation cases distribution functions are shown, see Figure 1.

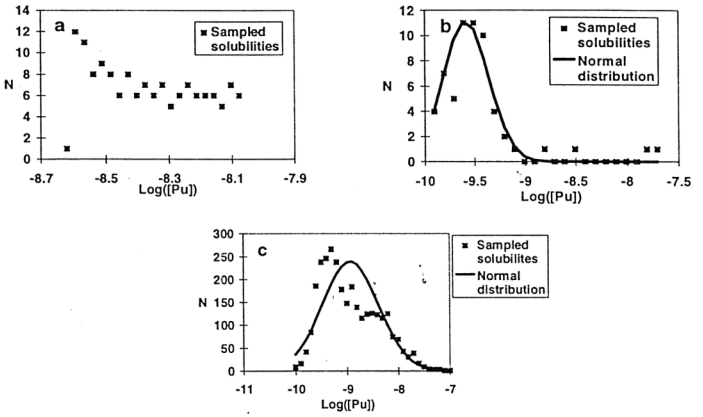

Figure 1, Distribution functions for three of the calculation cases,
a, isolated dissolution b, simulated water pumping
c, simulated random sampling

As seen in Figure 1 it is not obvious how the solubilities will be distributed for the different methods of solubility calculation. This implies that the use of the mean as the most probable value is not valid and therefore the distribution together with the maximum and minimum solubility gives the best information. For each of the cases the minimum and a maximum solubility is determined together with a confidence interval for the mean. In some cases, however, it may be difficult to fit the results to a well known distribution and therefore no attempt has been made to give a confidence interval based on the distributions but rather with one standard deviation calculated on logarithmic scale and then recalculated to linear-scale. This will naturally not produce a symmetric interval but the results are more easily read and the bias will shift the results to the higher end, thus making the results more concervative.

Table 1, Minimum and maximum solubility for the different calculation cases

	Isolated dissolution	one mineral	simulated water pumping	simulated random sampling
Solid phase	min ; max solubility	min ; max solubility	min ; max solubility	min ; max solubility
$Pu(OH)_2CO_3$	4.60E-12 ; 6.63E-12	1.41E-11 ; 2.19E-11	1.31E-12 ; 9.65E-12	1.13E-12 ; 4.43E-11
$Pu(OH)_4$	2.54E-09 ; 8.90E-09	1.09E-08 ; 5.39E-08	1.23E-10 ; 2.83E-08	9.72E-11 ; 2.75E-08

Table 1 shows that the variability between the different methods are far greater than their internal uncertainty except for the simulated random sampling. The latter covers almost the entire uncertainty space. Calculations have been made which show that the uncertainties in calculated solubility due to measurement uncertainties of the water composition, with the isolated dissolution model, are similar to the results obtained with simulated ground water composition uncertainties [9]. Uncertainty intervals of this magnitude have also been reported for a solubility calculation with the same water and database [10]. As comparison the minimum and maximum solubilities due to uncertainties in thermodynamic data for the $Pu(OH)_4(s)$ ranges some two orders of magnitude [5].

Table 2, Confidence intervals one standard deviation wide for the calculation cases

Solid phase	Isolated dissolution	one mineral	Simulated sampling	simulated random sampling
$Pu(OH)_2CO_3$	5.16E-12±5.17E-13	1.63E-11±2.44E-12	2.02E-12±9.08E-13	4.29E-12±3.05E-12
$Pu(OH)_4$	4.43E-09±2.03E-09	1.40E-08±2.18E-08	5.04E-10±8.36E-10	1.15E-09±8.38E-10

The great variation term in the simulated sampling case for $Pu(OH)_4$, seen in Table 2, originate from relative few samples and thus the outliers give a relatively large contribution to the variance.

7 CONCLUSION

When an attempt to model a real system is made, the uncertainties in the results due to selection of conceptual model are sometimes far greater than the uncertainties induced by uncertain input data. As a result, if several conceptual models exist it is important to examine the results from each of them before a large effort is made to determine the uncertainties in the simulated reality. Naturally this do not prevent that a sensitivity analysis ought to be made for each model to determine important parameters and other weak spots.

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AUTOMATIC DIFFERENTIATION FOR SENSITIVITY ANALYSIS. A TEST CASE.

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1 INTRODUCTION

The need for computation of gradients or jacobian is clear enough in sensitivity analysis and uncertainty evaluation for computer code calculation. Experience proves that computing partial derivative matrices, directly by finite difference approximation, is error prone, expensive and impractical for large scale systems. Using directional derivative finite difference approximation is less expensive but still sensitive to problem scaling and not accurate.

Automatic Differentiation is an easy, flexible, inexpensive and accurate way for getting derivatives. In this paper we present the use of the Automatic Differentiation tool `Odyssée` to compute gradients of `Thyc-1D`. `Thyc-1D` is a mockup of the industrial thermal-hydraulic in bundles code `Thyc-3D`. In a previous paper [1], we have shown some results using the two standard algorithms implemented for the direct or reverse mode of automatic differentiation on `Thyc-1D`. In this paper, we show some results using the two new algorithms for performing the reverse mode. This work was financed in part by EDF-DER and aims to the differentiation of `Thyc-3D` by `Odyssée`.

2 AUTOMATIC DIFFERENTIATION

Automatic differentiation is a set of techniques for computing derivatives at arbitrary points. Automatic differentiation is based on two main principles which are: a program can be seen as a composition of functions and can then be differentiated using the chain rule. The derivatives of elementary instructions are computed using standard rules for differentiating expressions such as: "the derivative of a sum is the sum of the derivatives" ...

Two modes of Automatic differentiation have been studied: the direct (or forward) mode that computes the derivatives and the initial values simultaneously, and the reverse (or backward) mode that computes first the initial values and then the derivatives in reverse order. The reverse mode is particularly efficient for computing gradients because its cost is independent from the number of inputs.

Any Automatic Differentiation Tool can compute directional derivatives or gradients. Two classes of Automatic Differentiation Tool exist: those which work source to source, and those which work by operator overloading.

`Odyssée`, `Adifor`, `Adjifor`, GRESS, `TAMC` belong to the first class of Automatic Differentiation Tools and work by code generation. In `Adifor` only the direct mode has been implemented. A new system called `Adjifor` (derived from `Adifor`) is under construction and implements the reverse mode. In GRESS and `TAMC` the two modes have been implemented. But they use strategies for storage/recomputation in reverse mode that do not make them applicable on large codes. The two main features of `Odyssée` are that it is able to differentiate a function even if some units have not been read by the system, and that a reverse mode applicable on operational codes has been implemented.

`Odyssée` (see [2] for the language reference manual) is an automatic differentiation tool developed at INRIA that differentiates Fortran-77 units. If a function is implemented as a set of units, `Odyssée` is able to differentiate it as a whole with respect to the inputs given by the user. From this set of units, `Odyssée` generates a new set of units that computes the derivatives. In `Odyssée`, the two modes of automatic differentiation have been implemented. In direct mode `Odyssée` uses the tangent linear algorithm to generate a Fortran-77 code that computes one directional derivative.

In reverse mode, one has to save (or recompute) all the variables modified by the initial function in order to compute the derivatives. The main drawback of the reverse mode is the size of this storage. In order to solve this problem, three different algorithms have been implemented in `Odyssée`.
In reverse mode, the code generated by `Odyssée` computes the cotangent code (equivalent to hand written adjoint codes) which is the product of a vector by the transposed jacobian.

Each generated units is composed of two parts: the forward part computes the trajectory and saves the modified variables, and the backward part restores the correct values of the variables and computes the derivatives. The standard cotangent linear algorithm (briefly described in [1]) saves statically any modified variable. It is based on the syntactical transposition of the code, and is only used to differentiate codes that contain only explicit loops (no `goto`). In the next two sections we shortly describe two new algorithms for the reverse mode.

The *flow inversion* algorithm extends the standard one and saves any modified variables but uses dynamic saves instead of static saves. It is based on the inversion of the flow graph and can then be applied to any code. The system extracts all the basic blocks from the code, then one execution of the code is equivalent to the sequence of all executions of the basic blocks. The system uses this property and saves the modified variables but also the indexes of the executed basic blocks in a pile, then the backward part is only the backward execution of the derivatives of the basic blocks with the corresponding restores. In the case of a general flow graph, the size of the saves can not be predicted, so the management of the execution pile must be dynamic and is done through some C code.

The *loop optimized* algorithm is based on a theoretical result described in [3] which aims at replacing in an "optimal way" the storage by recomputation. It uses an optimal strategy for replacing storage by recomputation in an explicit loop. If one calls *register* all the variables modified by the execution of one step of the loop, the user can chose the number of stored registers. During the forward part, only the initial value of the register is stored. During the backward part, the system computes the optimal step to save in order to minimize the storage-recomputation, and recomputes the intermediate steps. This algorithm, as for the initial one, can be only applied on routines which flow graph can be syntactically reverted (without *goto*, *stop*...). For example a *Do i=1, n* loop is reverted as *Do i=n,1,-1*.

3 ODYSSÉE APPLIED ON THYC-1D

In this paper, we will mainly describe the application of the reverse mode of `Odyssée` on `Thyc-1D`. `Thyc-1D` is a one dimensional thermal-hydraulic module for two-phase flow modeling. It consists of: three conservation equations for the two-phase mixture (mass, momentum and energy), one conservation equation for the vapor mass and one conservation equation for the relative liquid-vapor velocity between the two phases.

The aim of this study was to evaluate the sensitivity of the relative velocity between phases `ur` with respect to four parameters: `cd` and `qsi` included in the interfacial drag coefficient between vapor and liquid phases, `tau` the relaxation time in boiling modeling and `puisvol` the thermal power generated in the bundle.

In [1] we have shown on `Thyc-1D` the efficiency of the reverse mode of `Odyssée` in terms of execution time compare to tangent line but also to finite differences. But we have also shown the increase in terms of memory requirement. In this paper we will show the application of two new algorithms on `Thyc-1D`: the first on called *loop optimized* algorithm replaces storage by recomputation and uses static allocation for the derivatives and the saves, and the second one called *flow inversion* algorithm is based on the inversion of the flow graph contrarily to the two others and uses static allocation for the derivatives and dynamic allocation for the saves.

The target code `Thyc-1D` is made of three different kinds of routines; Fortran-77 routines, but also C routines, and routines from EDF's libraries as fluid thermodynamic properties. Those last two kinds of routines can not be read by `Odyssée`, therefore they are considered as black-box routines. In order to differentiate this code with `Odyssée`, we have built information bases that "replace" the definitions of the black functions. The system is then able to differentiate the whole function, but does not generate derivatives for those black-box routines. Their derivatives will have to be hand written using centered finite differences.

From `Thyc-1D`, we have generated four Fortran-77 codes with `Odyssée` using: the standard tangent linear algorithm (in direct mode), and the three different cotangent linear algorithms briefly described in the section above. Moreover, we have written by hand the derivatives of the black-box routines using centered finite differences with several steps (see [1] for more details). The first code (Thyctl) computes the gradient ($\frac{\partial ur}{\partial cd}, \frac{\partial ur}{\partial qsi}, \frac{\partial ur}{\partial tau}, \frac{\partial ur}{\partial puisvol}$) using four times the tangent linear code, the three other codes (Thyccl, Thyccl-opt, Thyccl-flow) compute in one shot the full gradient.

4 NUMERICAL RESULTS

We have compared the values of the derivatives given by the four codes (Thyctl, Thyccl, Thyccl-opt, Thyccl-flow), but also using optimal centered finite differences. We call optimal finite differences, the result obtained when the step-size is chosen to get the maximum of significant digits for each partial derivative. The three cotangent linear codes compute exactly the same values of the gradient. In Table 1, we show the values computed for the gradient of `Thyc-1D` with the tangent line (as reference) on line *tl*, the three generated codes in cotangent line on line *cl*, and by optimal centered finite differences on line *fd*.

One can see from the previous table that the numerical results given by the codes generated by Odyssée are the same, even if the Fortran-77 codes are really different (direct or reverse mode). At most, only the last 3 digits differ between the four codes. There is between 3 and 5 more correct digits using automatic differentiation than using finite differences.

Table 1: Comparison of gradients in double precision.

	$\partial ur/\partial cd$ D-00	$\partial ur/\partial qsi$ D-02	$\partial ur/\partial tau$ D-00	$\partial ur/\partial puisvol$ D-09
tl	−2.6877707476674	−1.1283833581385	0.23953473434534	8.4189731568450
cl	−2.6877707476678	−1.1283833581389	0.23953473434531	8.4189731568654
fd	−2.6877707	−1.1283833581	0.23953473	8.4189731

In this section, the *CPU* column gives the execution time in seconds, the *text* column gives the text length in bytes, the *stat. (dyn., total)* columns gives respectively the static (dynamic, total) size of the process at runtime. The column *ratio* shows the ratio between the values for the derivative and the same for the initial function.

The table 2 shows the execution time and memory requirement of the code generated in direct mode. The ratio in time is 2.12 less than the theoretical one which is 3.

Table 2: Comparison of execution time and memory space in direct mode

Thyc			Thyctl			ratio		
CPU	text	total	CPU	text	total	CPU	text	total
22.12	119	2082	47.02	199	2333	2.12	1.67	1.12

The Table 3 shows the different execution time, and size at runtime of the three codes generated in reverse mode. The results obtained using the initial algorithm have been described in [1], we recall it on the line 1 as reference. The line 2 shows the results for the *flow inversion* algorithm.
The lines 3, 4, 5, 6 show the results in execution time and memory requirement for the *loop optimized* algorithm, using different numbers of stored registers. The column labeled *reg.* shows the number of registers stored for the *loop optimized* algorithm.

Table 3: Comparison of execution time and memory space in reverse mode

line	code	reg.	cotangent line					ratio				
			CPU	text	stat.	dyn.	total	CPU	text	stat.	dyn.	total
1	Thyccl		157.61	441	18807	0	18807	7.1	2.3	9.0	0	9.0
2	Thyccl-flow		192.90	770	4736	16264	21000	8.7	6.5	2.3	7.8	10.1
3	Thyccl-opt	306	151.38	597	19015	0	19015	6.8	5.	9.1	0	9.1
4	Thyccl-opt	50	165.25	588	6228	0	6228	7.5	4.9	3.0	0	3.0
5	Thyccl-opt	10	179.17	588	4231	0	4231	8.1	4.9	2.0	0	2.0
6	Thyccl-opt	2	371.80	587	3831	0	3831	16.8	4.9	1.8	0	1.8

The second code is equivalent to the first one except that it uses dynamic allocation. It is a generalization of the standard algorithm to any Fortran-77 code. As with the initial algorithm the values of all the modified variables are stored. It uses a little more 2.3 than two times the initial static memory, and a little more total memory (for the execution pile). The dynamic memory represents the saves (copies of variables) necessary for the backward computation of the derivatives.

The values shown in the third, fourth, fifth and sixth lines come from the execution of the same Fortran-77 code (optimal linear cotangent code), but for different number of stored registers. In `Thyc-1D`, the main loop has been optimized. For our test case, the number of steps of this loop is 306. In line 3, the number of stored registers is 306, that means that the modified variables are stored at each step of the loop. The execution of this optimal code is then

equivalent to the execution of the two others codes, the execution time and memory requirement are then nearly the same. In the lines 4, 5, 6, the number of registers is less than 306 and decreases from 50 to 2. The memory requirement diminish-s and the execution time increases. The line 5 shows (for 10 stored registers the best compromise between execution time and memory requirement compared to the standard algorithm. One can see that the ratio in total size is 2 instead of 9 with the general algorithm whereas the ratio in time is 8.7 instead of 7.1. Such an algorithm is then really promising.

One must notice that those evaluation times do not depend on the size of the gradient (see [1]) for examples.

We are working on the application of `Odyssée` to `Thyc-3D` (see [4]). The cotangent line code of `Thyc-3D` generated with the third algorithm could not be run because of its size (93 Mega bytes). We intend to mix the two new algorithms introduced in this paper in order to be able to compute the gradients of `Thyc-3D` with respect to at least one hundred parameters.

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PARTIAL LEAST SQUARES (*PLS*) REGRESSION TO EXTRACT SIMPLE STATISTICAL RELATIONSHIPS FROM COMPLEX ENVIRONMENTAL MODELS

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1 INTRODUCTION

Models consisting of systems of deterministic equations play a prominent role in environmental research, and the merits of such models are indisputable. A substantial part of the modelling can be based on well-known scientific laws, and experimental studies can be designed to test the correctness of specific equations or submodels. Nevertheless, it may be difficult to comprehend the dynamic properties of complex models. For example, it is often practically impossible to trace the impact of natural fluctuations in climate through the different processes and compartments of a studied system. Hence, there is a strong need for procedures or tools that can extract simplicity out of complexity in environmental modelling [1].

The aim of the present study was to investigate if and how partial least squares regression or projection on latent structures (*PLS*) can be used to reveal the dominant modes of dynamic behaviour of deterministic models driven by daily climate data. We used *PLS* to examine *SOILN*, a process-oriented biogeochemical model developed to explain the loss of nitrogen from the root zone of arable soils [2]. Annual values of runoff and loss of nitrate from the root zone were regarded as response variables, and monthly values of climate variables, such as air temperature, precipitation and wind speed, were considered as explanatory variables.

2 MODELS AND DATA

2.1 The *SOILN* Model

The *SOILN* model [2] comprises a soil water and heat module [3] and a nitrogen module coupled in series. The water and heat module uses daily climate data (air temperature, cloudiness, precipitation, vapour pressure and wind speed) as input to predict soil water and heat conditions at any level in a soil profile; the main equations are derived from Fourier's and Darcy's laws, respectively. The nitrogen module includes the major processes determining inputs, transformations and outputs of nitrogen in arable soils. Nitrogen inputs can be in the form of commercial fertiliser or manure added to the top soil or as atmospheric deposition; harvest, leaching and denitrification constitute the outputs. The general structure of the *SOILN* model enables simulation of nitrogen losses from a wide variety of cropping systems. The model parameters used in the present study were selected to represent cultivation of barley on a sandy soil in southern Sweden.

2.2 Climate Data

Observed climate data comprised a 34-year-long series of air temperature, cloudiness, precipitation, vapour pressure and wind speed data from the city of Lund in southern Sweden. Synthetic climate data were generated in such a way that monthly mean values, variances, autocorrelations and cross-correlations in observed data were retained.

2.3 Partial Least Squares Regression

PLS is an indirect regression technique in which the variation of a response variable is linked to a large number of explanatory variables through a small or moderate number of factors that are defined as normed linear combinations of the explanatory variables. The first factor is selected to maximise the covariance with the response variable and is subsequently used as a regressor in an ordinary least squares regression (*OLS*) model. The next factor is selected to maximise the covariance with the estimated residuals from the *OLS* model. During the past decade, *PLS* has become a standard tool in chemometrics and multivariate calibration [4], and various theoretical aspects of the method have been investigated [5] - [10].

3 RESULTS

Values of the selected response variable, i.e., annual nitrate losses, were produced by feeding the *SOILN* model with *observed* or *synthetic* monthly climate data. Monthly climate data for the current and previous years were selected as explanatory variables in the *PLS* analysis. The results were presented as regression coefficients for standardised explanatory variables.

Figure 1 illustrates that the climate variables that had the greatest impact on the annual loss of nitrate were precipitation followed by cloudiness and air temperature. In addition, it was relatively easy to interpret some of the features of the temporal pattern in the estimated regression coefficients for monthly precipitation values. As expected, all regression coefficients for precipitation during the current year were clearly positive, whereas a wet autumn during the previous year seemed to slightly reduce the nitrate loss during the current year.

To further investigate the memory effects of past weather conditions, the *PLS* analysis was repeated using monthly records for the past four years. Figure 2 shows that such memory effects were mainly restricted to the conditions prevailing during the current and the previous year.

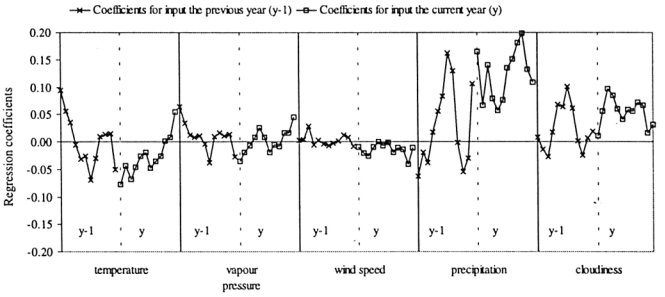

Figure 1: PLS analysis of the response in annual nitrate losses to monthly fluctuations in *synthetic* climate variables. The curve illustrates regression coefficients obtained by employing a one-factor PLS model to analyse data representing a time period of 400 × 30 years. The symbols y and y-1 respectively denote the current and the previous year.

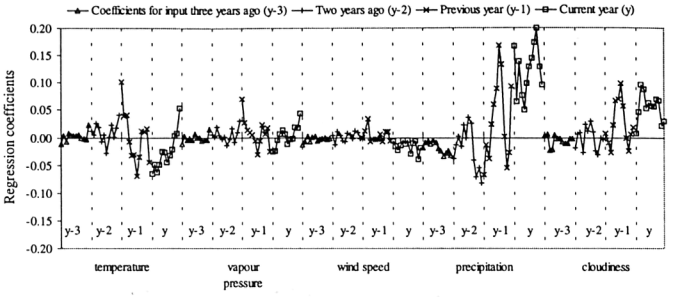

Figure 2: PLS analysis of the response in annual nitrate losses to monthly fluctuations in *synthetic* climate variables during the past four years. The curve illustrates regression coefficients obtained by employing a one-factor PLS model to analyse data representing a time period of 400 × 30 years.

Figure 3 shows a comparison of two *PLS* models, one based on 30 years of *observed* climate data (dashed line) and one based on 400 × 30 years of *synthetic* climate data (solid line). As can be seen, the large set of *synthetic* input data produced a pronounced pattern in the regression coefficients, whereas the coefficients obtained by using *observed* climate data exhibit more random variation. Closer examination of the regression coefficients obtained for different subsets of *synthetic* climate data showed that 30 years of such data is not enough to reveal the most influential input variables or the major time lags between input and output.

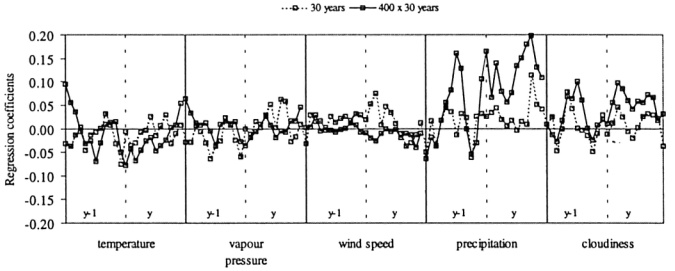

Figure 3: PLS analysis of the response in annual nitrate losses to monthly fluctuations in *synthetic* (solid line) and *observed* (dashed line) climate variables. The curve illustrates regression coefficients obtained by employing a one-factor PLS model.

Figure 4 shows a comparison of a one-factor *PLS* model and an ordinary least squares (*OLS*) model. The *PLS* model apparently provided more stable estimates of the regression coefficients than *OLS* did. However, in contrast to *OLS*, the estimates obtained by using *PLS* are not unbiased.

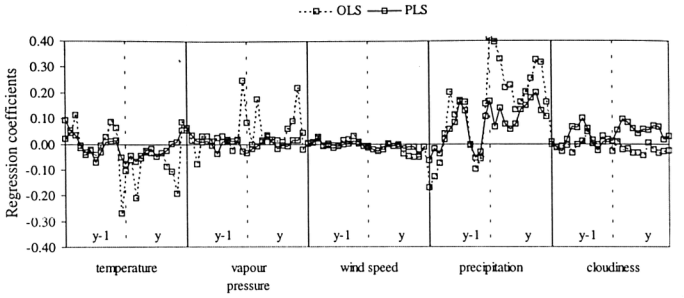

Figure 4: *OLS* and *PLS* analysis of the response in annual nitrate losses to monthly fluctuations in *synthetic* climate variables. Regression coefficients obtained by a one-factor *PLS* analysis (solid line) and by *OLS* analysis (dashed line) are shown.

CONCLUSIONS

The use of PLS enabled identification of the most important driving variables in the *SOILN* model and the major time lags between input and output. Long time series of artificially generated climate data were needed to reveal the dynamic behaviour of the studied model.

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SENSITIVITY ANALYSIS OF STEADY STATE RELIABILITY VARIABLES IN A TECHNICAL SYSTEM

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SUMMARY

RAM performance evaluation is considered for a ship electric propulsion system, based on Current Source Inverter (CSI) drive [1,2]. Steady state expressions of failure rate and repair rate for propulsion sub-systems are derived by the application of the Successive Reduction Method (SRM). Sensitivity analysis of these variables and of overall performance indexes (Reliability and Availability) is developed in two steps. First, the partial derivatives of the sub-systems repair and failure rates are computed with respect to the reliability parameters of the elementary components, following a conventional deterministic approach. Second, probabilistic properties of the system and subsystems performance indexes are evaluated against the distributions of the failure and repair rates of the sub-systems components. The results of Monte Carlo simulation is checked against the outcomings of the probability density functions, calculated on the basis of the partial derivatives as functions of two or more random variables. This procedure leads to an estimation of the risk and of the confidence intervals in evaluating overall performances, given the reliability parameters from the suppliers of the sub-systems [3,4].

Due to the high costs related to ship management [5] (investment, operational costs and maintenance costs), sensitivity analysis is very important to take account of the unavoidable dispersion of failure and repair rates extracted from data banks.

1 APPLICATION

A typical application requiring reliability assessment is electric ship propulsion drives (for cruise ships, icebreakers, several carriers and special purpose vessels); several realisations of electric propulsion systems are equipped with current source inverters (CSIs) feeding a synchronous motor (SM). A propulsion drive with two six pulse CSIs feeding a double star stator windings SM is shown in Fig. 1.

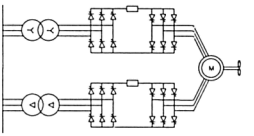

Fig. 1 Twelve pulse electric propulsion scheme

2 STEADY STATE RAM PERFORMANCES

2.1 Assumptions and methods

The study of ship propulsion system reliability and availability is based on the following assumptions:

- life time of the system is considered equivalent to the mission time (MT), since the maintenance performed at the end of each mission allows to neglect the ageing (the system is periodically brought back to the initial performances);
- system mean time to failure (MTTF) is assumed and verified to be longer than MT.

The study is performed considering:

- the identification of the reduced structural functional layout and the assessment of the failure rate λ_i and repair rate μ_i of each elementary component or equipment (according to the "smallest replaceable unit" rule);
- the application of the successive reduction technique (SRM) to the whole system;
- the development of uncertainty and sensitivity analysis (SA) of the equivalent failure and repair rates.

2.2 System Reduction

A successive reduction technique (SRM) is developed; each subsystem having a series or parallel configuration from the reliability point of view is replaced by an equivalent component using the following relationships [1].

For the series connection of K components the equivalent λ_s and μ_s are obtained:

$$\lambda_s = \sum_{i=1}^{K} \lambda_i \qquad \mu_s \approx \sum_{i=1}^{K} \lambda_i \Big/ \sum_{i=1}^{K} (\lambda_i / \mu_i) \tag{1a,1b}$$

For the parallel connection of K components the equivalent λ_p and μ_p are obtained:

$$\lambda_p = \left[\sum_{i=1}^{K} \mu_i\right] \cdot \left[\prod_{i=1}^{K} (\lambda_i / \mu_i)\right] \qquad \mu_p = \sum_{i=1}^{K} \mu_i \tag{2a,2b}$$

Approximate expressions (1b) and (2a) are derived assuming that mean time to failure is larger than mean time to repair (MTTF>>MTTR). Hence, this assumption, when the failure and repair rates of each component are considered, implies that

$$\frac{\lambda_i}{\mu_i} << 1 \tag{3}$$

due to the lack of memory of the exponential model (λ=1/MTTF and μ=1/MTTR) [1].

SRM applied to the electrical system leads to a block diagram synthesis, composed of series and parallel connected subsystems (see Fig. 2); for the electric ship propulsion system three subsystems can be identified: S_1 *AC/AC conversion subsystem*, S_2 *AC drive hardware and digital control subsystem*, S_3 *SM and exciter subsystem*). The most critical subsystem S_1 is considered, which corresponds to the series configuration S_s (see Fig. 2(a)); the parallel configuration S_p with the same 5 components is included for comparative analysis.

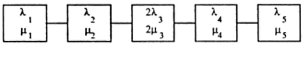

Fig. 2(a) Series reference system

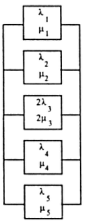

Fig. 2(b) Parallel reference system

Table 1 Failure and repair rates of reference S_s and S_p systems (FIT = $[10^9\ \text{hr}]^{-1}$)

Subsystems	Components	λ [FIT]	μ $[\text{hr}]^{-1}$
Series and parallel systems	Circuit breaker	λ_1=100	μ_1=0.25
	Transformer	λ_2=900	μ_2=0.0054
	Six pulse converter	λ_3=5400	μ_3=0.25
	Reactor	λ_4=10	μ_4=0.01
	Hardware Module	λ_5=4000	μ_5=0.25

3 SENSITIVITY ANALYSIS

Sensitivity analysis (SA) of the system reliability and availability functions is performed in two steps. First, the partial derivatives of the sub-systems repair rates μ_{Si} and failure rates λ_{Si} are computed with respect to the reliability parameters of the elementary components, following a conventional deterministic approach. Second, probabilistic properties of the λ_{Si} and μ_{Si} are evaluated against the possible statistical distributions of the elementary components λ_i and μ_i, considered at the previous step.

3.1 Deterministic evaluation by means of partial derivatives

The partial derivative of the expressions for equivalent λ and μ of series and parallel connections (1) and (2) with respect to the failure rate λ_i and repair rate μ_i of the i-th elementary component gives the relationships (4a,b,c) and (5a,b,c).

$$\frac{\partial \lambda_s}{\partial \lambda_i} = 1 \qquad \frac{\partial \mu_s}{\partial \lambda_i} = \frac{1 - \mu_s/\mu_i}{\sum_{j=1}^{K} (\lambda_j / \mu_j)} \qquad \frac{\partial \mu_s}{\partial \mu_i} = \frac{\lambda_i}{\mu_i^2} \frac{\mu_s}{\sum_{j=1}^{K} (\lambda_j / \mu_j)} \tag{4a,4b,4c}$$

$$\frac{\partial \mu_p}{\partial \mu_i} = 1 \qquad \frac{\partial \lambda_p}{\partial \lambda_i} = \frac{\lambda_p}{\lambda_i} \qquad \frac{\partial \lambda_p}{\partial \mu_i} = \lambda_p \left(1 \Big/ \sum_{j=1}^{K} \mu_j - \frac{1}{\mu_i} \right) \tag{5a,5b,5c}$$

Eq. (5b) and (5c) have been obtained by direct substitution of (2a). Eq. (4b,c) and (5b,c) are analysed for two extreme cases: large and small λ_i/μ_i ratios, holding eq. (3).

Equation (4b)

Considering (4b), for large λ_i/μ_i ratio the relationship may be simplified to a nearly hyperbolic function, whose primitive is

$$\mu_s \equiv c_1 - c_2 \mu_i \ln(\lambda_i) \tag{6}$$

which shows a slope change for particular λ_i and μ_i values. The μ_i value which gives a null derivative is sought for two cases: first, when there are only two significant λ_i/μ_i ratios (λ_1/μ_1 and λ_2/μ_2) the solution is directly $\mu_1=\mu_2$; second, when there are three significant λ_i/μ_i ratios (λ_1/μ_1, λ_2/μ_2 and λ_3/μ_3) the solution is either $\mu_1=\mu_2=\mu_3$ or the more general $\mu_1+\mu_2=2\times\mu_3$.

For small λ_i/μ_i ratio the relationship may be simplified as

$$\frac{\partial \mu_s}{\partial \lambda_i} = \frac{1}{const.} \left[1 - \frac{1}{\mu_i} \frac{1}{const.} \sum_{j=1}^{K} \lambda_j \right] \tag{7}$$

The value of (7) for the smallest λ_i/μ_i ratio can be considered constant as a function of λ_i, even if the numerator depends on λ_i too.

Equation (4c)

For large λ_i/μ_i ratio (4c) is independent on μ_i and μ_s is a linear function of μ_i (eq. (1b) is plotted in Fig. 3).

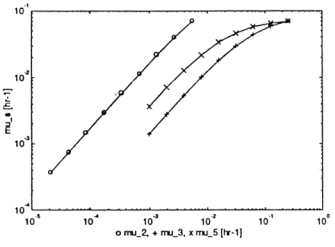

Fig. 3 μ_s as a function of μ_2, μ_3 and μ_5 (the three largest λ_i/μ_i ratios)

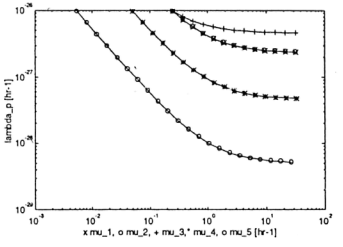

Fig. 4 λ_p as a function of μ_1, μ_2, μ_3, μ_4 and μ_5

For small λ_i/μ_i ratio eq. (4c) may be approximated as

$$\frac{\partial \mu_s}{\partial \mu_i} = \frac{\lambda_i}{\mu_i^2} \mu_s \tag{8}$$

Eq. (8) leads to the exact solution

$$\mu_s = c_1 \, e^{-\lambda_i/\mu_i} \tag{9}$$

which is nearly constant for practical λ_i and μ_i values. If μ_1 and μ_4 are considered, it can be stated that μ_s is unaffected (the variation is approximately 0.1%) by a change of two order of magnitude of their value.

Equation (5b)

Considering (5b), λ_p is a linear function of λ_i whatever the value of the λ_i/μ_i ratio.

Equation (5c)

Eq. (5c) may be simplified for all values of the λ_i/μ_i ratio as

$$\frac{\partial \lambda_p}{\partial \mu_i} = -\frac{const\ \lambda_i}{\mu_i^2} \tag{10}$$

which leads to the exact solution (eq. (2a) is plotted in Fig. 4)

$$\lambda_p = \frac{const\ \lambda_i}{\mu_i} \tag{11}$$

3.2 Probabilistic evaluation based on data uncertainty

According to the results obtained by a classical study using the partial derivative of the reliability performance formulation, a probabilistic analysis could be developed. Uniform probabilistic distribution functions of λ_i and μ_i are assumed and the probability distribution of the subsystems failure and repair rates are analysed as far as the series and parallel connections are concerned [6]. The results of the Monte Carlo simulations are given in Fig. 5–8. Attention has been focused on the component 2 (transformer) of S_s and S_p: λ_2, μ_2 and μ_4 range is 400÷1400 FIT, 0.0014÷0.0094 hr^{-1} and 10^{-4}÷0.1 hr^{-1}.

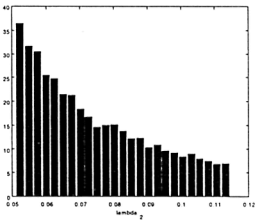

Fig. 5 Pdf of μ_s as a function of λ_2 (unif. distr.)

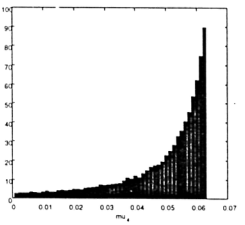

Fig. 6 Pdf of μ_s as a function of μ_4 (unif. distr.)

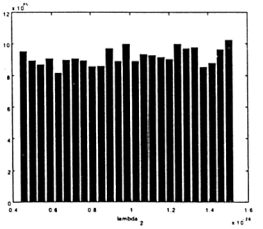

Fig. 7 Pdf of λ_p as a function of λ_2 (unif. distr.)

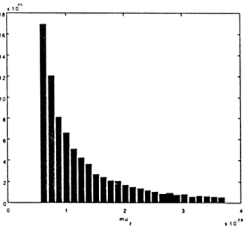

Fig. 8 Pdf of λ_p as a function of μ_2 (unif. distr.)

The pdf shown above are in accordance with the considerations made and the approximate relationships drawn in section 3.1 for uniform pdf of λ_2 and μ_2. The following consideration are valid for uniform pdfs of λ_2 and μ_2.
The pdf of μ_s as a function of λ_2 (Fig. 5) is exponential as indicated by (6); further investigation is necessary to assess the correct relationship.
The pdf of μ_s as a function of μ_3 (Fig. 6) may be splitted into three parts: quasi-uniform for small values (μ_s behaves linearly); nearly hyperbolic as it can be desumed from Fig. 3; approximate delta distribution centred on the asymptotic value of μ_s.
The pdf of λ_p as a function of λ_2 (Fig. 7) is a uniform distribution as it was stated in section 3.1 Equation (5b).
The pdf of λ_p as a function of μ_2 (Fig. 8) is hyperbolic as indicated by (11).

4 CONCLUSIONS

The probabilistic analysis by means of Monte Carlo simulation (section 3.2) confirmed the results of section 3.1, based on partial derivatives and differential equation solution, and may be extended to the evaluation of the pdfs of subsystem failure and repair rates as a function of multiple random variables (the components failure and repair rates). Further investigation may be performed for pdf other than uniform, noting that generally, failure and repair rates of system components are given as either (min, max) or (average, confidence interval) values, indicating the former a uniform distribution and the latter a normal distribution for data dispersion [2, 3, 4].
SA is a valid tool to assess the influence of parameters uncertainty on the overall system failure and repair rates and to identify the most critical parameters, to be acquired more precisely by means of for instance a more detailed analysis of reliability databases.

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SENSITIVITY ANALYSIS AND UNCERTAINTY MODELLING IN DECISION SUPPORT SYSTEMS

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1 INTRODUCTION

In [[1] French and Liang proposed the following definition:

> A *decision support system* is a computer-based system which helps decision makers form and explore the implications of their judgements and hence to make a decision based upon understanding.

There are many other definitions of decision support systems (DSS), many of which allow the inclusion of almost any information system, but the discussion in this paper is limited to DSS's which focus their support on the evolution of judgement: i.e. which implement aspects of *prescriptive* decision analysis (Figure 1). The purpose of such analyses are discussed in [[1] and [[2].

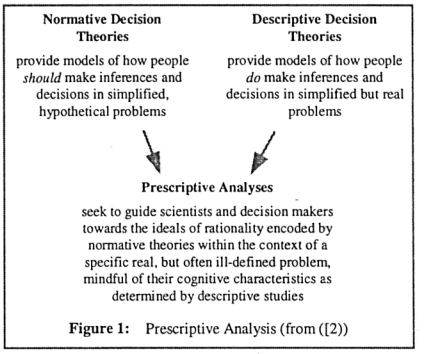

Figure 1: Prescriptive Analysis (from ([2))

What are the implications of this interpretation of DSS's for the sensitivity analyses and uncertainty analyses included in such systems? Both seek to address and inform the decision makers' judgements of belief and uncertainty. When should the system provide the means for analysing models of uncertainty and when should it allow the decision makers to explore uncertainty through sensitivity analysis? This paper seeks to address these questions, drawing examples from the RODOS, a DSS for nuclear emergencies [4].

2 UNCERTAINTY MODELLING AND ANALYSIS

In many points in a decision analysis one represents uncertainty through probability: at least one does, if one accepts the principles of rationality underlying the Bayesian School (Figure 2). For the purposes of this paper, such an acceptance will be assumed. These probabilities are built into probability models which encode relations and dependencies between the decision makers' beliefs and uncertainties. As data arrive, applications of Bayes' Theorem in the analysis of the model prescribe how the beliefs should be updated. Bayesian updating provides the decision makers with guidance on the import of data and how they should be assimilated into their beliefs. Note that the Bayesian methodology separates issues of (scientific) knowledge from the value judgements needed to make a decision, the latter being modelled with multi-attribute utility models (MAUT): see, e.g. [[2].

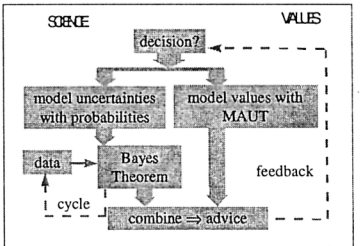

Figure 2: Bayesian analysis

3 DEALING WITH UNCERTAINTY IN DECISION SUPPORT

In [6] several 'categories' of uncertainty that arise in a decision analysis were discussed. There seem to be three responses to the need to address uncertainty:

1. model and analyse the uncertainty;
2. discuss the issue and resolve ambiguity through clearer understanding;

3. investigate the sensitivity of the output to input judgements about which the decision makers are uncomfortable.

These responses will be explored in the following, taking the RODOS system as an example.

4 RODOS

The RODOS system (**R**eal time **O**nline **D**ecisi**O**n **S**upport) is designed to be a decision support system (DSS) for off-site nuclear emergency management, capable of finding broad application across Europe [4]. It is intended to be comprehensive and integrated (i.e. applicable at all distances from the release and over all times for which countermeasures may need to be taken to mitigate the consequences of an accident). It must necessarily support many groups of decision makers from local emergency managers to national and international political decision forums. In designing RODOS, many aspects of uncertainty modelling and sensitivity analysis are being addressed. There is a clear need to think clearly about the modes of analysis that will be supported.

5 THE MODELLING OF UNCERTAINTY WITH RODOS

In order to deal with the uncertainty inherent in managing a nuclear accident, techniques are being incorporated into RODOS to support consideration of the following [7], 8]:

- Will there be a release (given that a 'trip' has occurred in the reactor)?
- What is/will be the source term (composition, time behaviour, and release co-ordinates including height)?
- How might the weather conditions develop, especially when and where might there be precipitation?
- What observation errors are in any monitoring data, including the possibility of human error?
- What is the quality of the meteorological, hydrological, agricultural, health and economic models to be used?
- What will be the level of success in implementing any protective measure, including public compliance with advice?
- What is the demography of the affected population and where are they at the moment?
- What is the accuracy of approximations used in calculations?

These uncertainties relate to the decision makers' lack of knowledge. Incoming data may resolve or reduce some of these uncertainties. Notice that data assimilation and the handling of uncertainty are intimately connected. To understand the import of data, one needs to understand the relative uncertainty in the current predictions relative to the current data. Equally to understand the uncertainty in a prediction from a model, one needs to have an understanding of the quality of the data and judgement on which it is built. Some of this understanding is built using Monte Carlo analyses and comparative studies *before* an accident to gain an intuition for the predictive of quality of the models generally (see, e.g. [[9]). During the course of the accident, data assimilation and model checking techniques may be used both to improve the predictions, where possible, and to warn the user when the models seem to be departing seriously from the real situation. Within RODOS, we are using a variety of techniques from belief nets to krigging to assimilate many types of data including:

- plant status data;
- meteorological data;
- on-site stack and periphery monitoring data, off-site fixed and mobile monitoring data;
- hydrological data concerning both flow rates, depths, etc. and contamination;
- demographic data concerning the groups liable to be exposed;
- agricultural, economic and land use data;
- data on compliance with and effectiveness of countermeasures.

Some data are obtained by measurement, the statistical characteristics of which are reasonably well known; but others are derived from expert judgement, the statistical characteristics of which are less clear and very different [12]. But, none the less, the Bayesian methodology can cope – in principle – with all the data, although the technical difficulty of doing so is considerable. Note that these analyses correspond with activities on the left hand side of Figure 2 and correspond to the first response noted in section 0.

Turning to the second response of section 0 and the right hand side of Figure 2, decision makers are often uncertain about their objectives and how to evaluate the consequences. How should they deal with such matters as 'equity' or 'public acceptability'? These uncertainties relate to value judgements. French [[8] has argued that such uncertainties can only be reduced by discussion and clear thought. One cannot derive values judgements from data analysis. One must explore with the decision makers what they mean by their nebulously defined objectives, help them clarify them and articulate them in operational ways [[11, 13]. Lack of clarity on objectives and the articulation of other concepts in a decision analysis is often described not by the term 'uncertainty' but by 'imprecision'. Many authors have suggested that imprecision may and should be modelled by techniques such as fuzzy sets. But if the purpose of decision analysis and decision support is to help the decision makers *understand* the issues and so make a better decision through this understanding, then it is hard to see how modelling imprecision as opposed to resolving it can help [6]. Whereas within decision analyses conducted under normal timescales one can use 'soft' OR techniques to help formulate and develop the objectives and attributes (see, e.g. [14, 15]), within the early phases of emergency management there is not enough time to do so. Thus there are

many activities associated with the development of the RODOS system and elsewhere in nuclear safety to determine objectives and other value judgements in preparation for an accident [16]. Sadly but perhaps not surprisingly, one of the findings of these exercises is that the decision makers are very discomforted by being confronted with uncertainty. It is clear that we need better methods of communicating uncertainty and preparing the decision makers to deal with it.

6 SENSITIVITY ANALYSIS

The third response of section 0 was that to address some uncertainties we need to investigate the sensitivity of the output to input judgements about which the decision makers are uncomfortable. It is easy on reading presentations of Bayesian methods to assume that with sufficient introspection all judgemental inputs may be defined to whatever accuracy is necessary, whether they refer to parameters in probability distributions or weights and utility values in MAUT methods. But such is not the case. The idealisation of rational economic man with infinite discrimination and introspective power at the centre of the normative theory does not match the abilities of human decision makers. They will always be uncertain about some inputs, being able to define a parameter, correlation, weight or whatever to within a rough range but not to many significant figures. The term 'rough range' should not be interpreted in any technical sense. One cannot define an interval with hard endpoints, a fuzzy membership function or any other quantification without entering an infinite regression. It simply means that the decision makers judge quantities to be "about x%" or whatever: no more. Sensitivity analysis provides the means of addressing this uncertainty and it also provides rather more. To appreciate the full significance of its role three perspectives are valuable:

The Technical Perspective. This is the investigation of the effect of changes in the data input to a model on the output of that model. It helps the decision makers explore whether there is a clearly preferred alternative, or whether there are several strongly competing alternatives [[17].

The Cognitive or Individual Perspective. Sensitivity analysis is an interactive exploration of the effects of changes in the inputs to and structure of a model in order that the decision makers may learn about the problem and about their judgements. The viewpoint here is the growth in understanding of each individual decision: see, especially, the concept of requisite decision analysis [[11].

The Social or Group Perspective. Sensitivity analyses can help groups of decision makers focus on their *real* differences. Often a heated and fundamental disagreement can be completely defused by a sensitivity analysis which shows that, despite differences between their individual judgements, the decision should be the same. In this way sensitivity analysis contributes to group communication and the building of a shared understanding [[11].

Within the RODOS system, the design of the evaluation subsystem recognises all three roles of sensitivity analysis [4, [8, 16]. However, we have still to address the issues fully within the predictive modules, where the computational problems are considerable and we have also to contend with the reluctance of the decision makers to tackle uncertainty head on. There is much work to be done.

7 CONCLUDING REMARKS

In the above, the focus has been on uncertainty issues in decision support for emergency management as embodied in the design of RODOS. The ideas can be translated *mutatis mutandis* to support for many one-off decisions; but of course the emphases will change. Moreover, the terminology varies between different areas of application. For instance, in risk assessment either for design studies or licensing decisions there is usually much more time to conduct an analysis: time for extensive what-if and Monte Carlo analyses in which the inputs are varied. This variation may be conducted in two ways:

- Stochastic variation. Here the analyst's confidence in an input value, *viz.* data point or parameter, can be encoded by means of probabilistic measures: ideally a full distribution, but often only quantiles or variances (and other moments) are available. In this case the inputs are varied stochastically in Monte Carlo analyses and the resulting distribution of the outputs studied. This is an archetypal example of *uncertainty analysis*, as it is know in risk assessment. It addresses uncertainty in the sense of the first response: see Table 1.
- Deterministic variation. Here the analyst has no guidance to the confidence in the input value available in a probabilistic form. Maybe there are bounds upon the 'permissible' values and thus deterministic calculations may be undertaken to see the range of outputs which may arise from input values in the permissible range. This is an archetypal example of sensitivity analysis, as discussed in section 0 above. It addresses uncertainty in the sense of the third response: see Table 1.

In summary, there are three ways to address uncertainty in decision support and we need to be clear on the appropriate use of each.

Table 1: Methods of addressing uncertainty

Method of Addressing Uncertainty		Techniques
Model and analyse the uncertainty	↔	probability modelling and uncertainty analysis
Discuss the issue and resolve ambiguity through clearer understanding;	↔	soft OR and problem formulation techniques
Investigate the sensitivity of the output to input judgements about which the decision makers are uncomfortable.	↔	sensitivity analyses

8 ACKNOWLEDGEMENTS

The RODOS system is being developed by a consortium of many institutes from across Europe and the Former Soviet Union with support from the European Commission's Framework R& D programmes under contracts F14P-CT95-0007, F14C-CT96-0006, IC15-CT96-0318. I am grateful to all my colleagues in the project, especially my co-workers Nadia Papamichail, Kostas Politis, David Ranyard, and Jim Smith. However, the views expressed here are mine and do not necessarily reflect those of the RODOS project. I am also grateful for many discussions with Roger Cooke, Tim Bedford and the ESSRDA Uncertainty Analysis Working Group.

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SENSITIVITY ANALYSIS BASED VARIABLE SELECTION IN LINEAR REGRESSION AND NEURAL MODEL IDENTIFICATION A CASE STUDY IN SHORT-TERM ELECTRIC PEAK LOAD FORECASTING

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In this paper, a methodology for - sensitivity analysis based - variable selection in casual forecasting model identification is presented on the basis of case study in next-day electric peak load forecasting. The methodology is based on the concepts of W.Milo [7, 3] and A. P. Refenes, A. D. Zapranis, and J. Utans [12].

Next-day peak load forecasting plays important role in various power system applications such as economic dispatching of generation units and possible energy interchange with other utilities [Onoda '94]. In prior research, several techniques have been studied for peak load forecasting, including approaches of regression, neural nets [9, 2], expert networks [1].

The load time series are complex and non-stationary. The load consist of daily, weekly, and annual cycles. So as to examine the embedded periodicity in the load trend and reliably determine the necessary historical load data, we introduced the ARIMA procedure. The study indicates, that the load data from previous day, and the same day of the previous week are required.

There are reported in the literature successes in introducing weather indicators to the practice in load prediction [9, 4]. The peak of the daily load is strongly influenced by the recent weather conditions. This concerns: temperature, humidity, wind velocity, sky condition.

In our research, evening peak load value at time t (EP_t) is computed on the basis of the values of several weather variables at time t and t-1 ($WI_{i,j}$, $i \in \{t,t-1\}$, and j indicates weather indicator), evening peak load values at time t-1 and t-7 (EP_k, $k \in \{t-1,t-7\}$), and morning peak load value at time t (MP_t). Daily data (concerning morning, noon, and evening values) was considered in the model, and the total sample data (training data) covers the period from 1st January 1992 to 31st December 1992 and the total out-of-sample data (testing data) covers the period from 1st January 1993 to 31st December 1993.

The task is to select variables from the universe of weather variables (WI_t, WI_{t-1}) of the inicial model described as follows:

$$EP_t = \varphi\,(EP_{t-1}, EP_{t-7}, MP_t, WI_{t,j}^{m}, WI_{t-1,j}^{m}, DW_t)$$

where:

t indicates the forecasting day;
j, j=1..4, indicates weather variable, and j=1 is temperature value, j=2 is humidity value, j=3 is wind value, and j=4 is cloudiness value;
m indicates part of the day, and m=1 is morning, m=2 is noon, and m=3 is evening indicator;
DW is a vector of dummy variables concerning the day of the week.

The functional relationship (φ) between evening electric peak load value and variables specified in the model is tested for the two models: linear (multiple linear regression model) and non-linear (neural network model). Having tested linear relationship, it was considered the model as follows:

$$EP_t = \beta_0 + \beta_1 EP_{t-1} + \beta_2 EP_{t-7} + \beta_3 MP_t + \beta_j^{m} WI_{t,j}^{m} + \beta_j^{m} WI_{t-1,j}^{m} + \beta_n DW_t + \varepsilon,$$

where m=1..6, and ε represents non-predictable part of the evening electric peak load forecast value, i.e. the error of the model and β-s are the free parameters of the linear model.

Having tested non-linear relationship, it was considered the model as follows:

$$EP_t = g\,(EP_{t-1}, EP_{t-7}, MP_t, WI_{t,j}^{m}, WI_{t-1,j}^{m}, DW_t, W) + \varepsilon$$

where g is a neural estimator of the φ and W is a set of free parameters of the neural model, i.e. connectionist weights, and $W = \{w_1, w_2, ..., w_p\}$, and p is constant.

For the models specified above, the multiple linear regression is introduced so as to obtain estimators of the parameters β and back propagation learning rule is introduced so as to obtain estimators of the free parameters of the neural model.

Weather variable selection is performed in the backwards stepwise procedure, separately for the two models, i.e. the multiple linear regression and the multi-layer perception like neural network model with back propagation learning algorithm, on the basis of the analysis of linear model stability (numerical and statistical) [7, 3] for the first model and statistical significance estimation [12] for the second model. The procedure starts by including all weather variables and then deleting variables one at the time. The criterion for deleting variables is to select the ones, which reduces the percentage error the most.

The selected weather variables are then used to forecast out-of-sample (i.e. testing) electric evening peak load. The computations are performed for the two models: the multiple linear regression and the multi-layer perception like neural network model with back propagation learning algorithm, and the performance of the models are compared through the forecasting percentage error.

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SENSITIVITY ANALYSIS FOR AN ENVIRONMENTAL RISK ASSESSMENT METHOD

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During last years, the concept of risk has been applied increasingly in environmental problems; in fact, risk links the occurrence probability of an harmful event to its adverse effects.
Many environmental standards and criteria are established as threshold values which can not be exceeded to keep safe the contamination targets; for example, in water pollution control problems, large concerns are about dissolved oxygen, nutrients and toxic substances levels which must have values compatible with the ecosystem components.
Therefore, the concept of risk could be used in order to characterize the occurrence probability of incompatible values of water quality parameters and the dimension of their adverse effects on the aquatic ecosystem components; thus, the potential of these for survival could be assessed.
Particularly, beginning from the distribution of some water quality parameters, we could know the probability of qualitative standards violation; thus, if we are also able to predict the effects of this violation for the ecosystem, we could assess the risk.
In this approach, the application of a water quality model is very useful; in fact, this model could provide reliable predictions of water quality parameters values in the water body for different situations. Thus, comparative risk assessment could be performed.
In a former paper, a risk assessment method based on first and second order moments was applied in order to evaluate the death risk for fish due to unacceptable levels of dissolved oxygen and free ammonia in a river downstream of a wastewater treatment plant without nitrification. Thus, environmental risk reduction in the river due to the introduction of nitrification in the plant was predicted [1].
Generally speaking, this method is based on comparison between contaminant level C and contamination resistance of the fish R; both C and R are assumed as random variables with known mean, standard deviation and distribution. Therefore, the method requires the knowledge of these probability parameters [2].
In our case, the method was applied to daily DO_{min} and free ammonia FNH_3 which were modeled, together with dissolved oxygen need for fish survival R_{DO} and free ammonia resistance R_{FNH3}, as a random variables with normal distribution. Thus, the means μ_{DO}, μ_{FNH3}, μ_{RDO} and μ_{RFNH3} and the standard deviations σ_{DO}, σ_{FNH3}, σ_{RDO} and σ_{RFNH3} had to be known.
The water quality data for DO_{min} and free ammonia were obtained from simulation with USEPA's model WASP 4.32 [3], which has been formerly calibrated and verified for the river [4] [5]; therefore, mean and standard deviation for DO_{min} and free ammonia were obtained performing a model sensitivity analysis through a simple input parameter perturbation [6]; the parameters involved in perturbation were kinetic coefficients such as the carbonaceous BOD decomposition rate K_{CBOD}, in 1/days, the nitrogenous BOD decomposition rate K_{NBOD}, in 1/days, the reaeration rate K_a, in 1/days, and the photosyntethic production and respiration P and R, in mg O_2/liter×day [7]. Particularly, the perturbation ranges were set equal to standard deviations of each kinetic parameters.
These perturbations result in DO_{min} and FNH_3 variations, which represent the standard deviations of DO_{min} and FNH_3 for each perturbation; thus, these variations were called σ_{Ka}, σ_{Kcbod}, σ_{Knbod}, σ_P and σ_R, respectively. Finally, the overall standard deviations σ_{tot} for DO_{min} and for FNH_3 were obtained through the following relationship [8]:

$$\sigma_{tot} = \sqrt{\sigma_{Ka}^2 + \sigma_{Kcbod}^2 + \sigma_{Knbod}^2 + \sigma_P^2 + \sigma_R^2} \qquad (1)$$

First and second order moments for R_{DO} and R_{FNH3} were defined on available literature data basis.
In fact, many studies have been performed about fish mortality for hypoxia and free ammonia [9] [10]; usually, in chemicals toxicity studies, test results are expressed through the so-called 96-LC_{50}, i.e. lethal concentration for the 50% of the individuals after 96 hours of exposure.

There are few available data of 96-LC_{50} for DO; thus, expressing fish and, more generally, aquatic life resistance through a criterion based on a simple minimum allowable DO concentration is considered the most practicable approach in river management [10].

Many data are available for free ammonia; however, generally speaking, the fre ammonia 96-LC_{50} values are affected by DO levels, temperature, pH, acclimation and fluctuating exposure, carbon dioxide, salinity and presence of other chemical [9]; furthermore, 96-LC_{50} may vary among different fish species.

Therefore, in a simpler way, μ_{RDO} and μ_{RFNH3} were set equals to the italian water quality mean thresholds values of 5.0 mg/l and 0.025 mg/l, respectively.

The values for standard deviations σ_{RDO} and σ_{RFNH3} were another critical points for lack of available data. Thus, it seemed to be advisable to perform a sensitivity analysis for those parameters to get a deeper insight into the method; therefore, σ_{RDO} and σ_{RFNH3} were varied within a range of 10÷50% with a variation step of 10% .

For non-nitrified effluent, death risk $p_{d\text{-}DO}$ is always very high; particularly, it is always over 50% and it is mostly over 90%. A σ_{RDO} increase results in a reduction, up to 20% (Fig.1a); on the contrary, for nitrified effluent, higher values for σ_{RDO} corresponds to higher death risk almost along all the river. However, in central reaches, death risk value is slighty affected by σ_{RDO} value (Fig.1b).

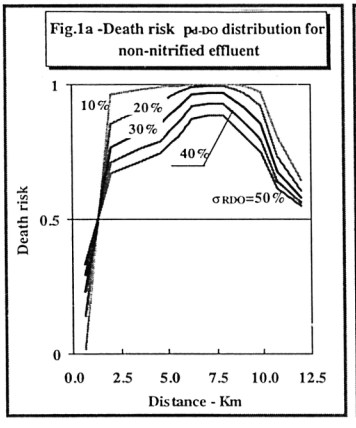
For non-nitrified effluent, death risk $p_{d\text{-}FNH3}$ is always near 100%; it is reduced to 80% only when σ_{RFNH3} increase to 50% (Fig.2a). For nitrified effluent, near the wastewater treatment plant discharge the death risk $p_{d\text{-}FNH3}$ is higher for σ_{RFNH3} lower values, while in the final reaches of the river the contrary occurs (Fig.2b); furthermore, death risk appears to be remarkably affected by σ_{RFNH3} value. Then, it should be noted that at the abscissa 5.1 Km, $p_{d\text{-}FNH3}$ is the same for each σ_{RFNH3} value (Fig.2b).

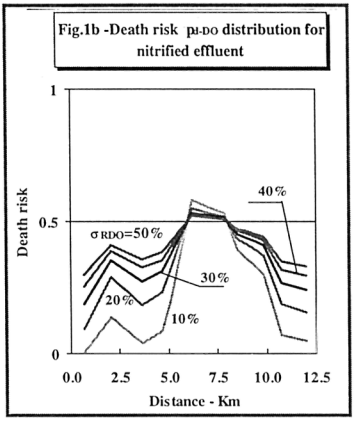
Finally, the total death risk $p_{d\text{-}tot}$ is always over 90% for non-nitrified effluent; it is slighty affected by σ_{RDO} and σ_{RFNH3} value (Fig.3a). In-plant nitrification results in a remarkable $p_{d\text{-}tot}$ reduction (Fig.3b); σ_{RDO} value appears to have a great influence on risk levels, exspecially in the final reaches of the river, where, for σ_R=50% and σ_R=10%, $p_{d\text{-}tot}$ is 50% and 5%, respectively.

Generally speaking, for nitrified effluent, higher σ_R values results in lower death risk distribution variability while lower σ_R values results in a wider range of death risk levels.

Furthermore, the distributions appear to invert their shapes at definite death risk values, i.e. 50% for single risk and 75% for total risk.

In conclusion, the sensitivity analysis performed has pointed out the relevant influence of σ_{RDO} and σ_{RFNH3} parameters values on environmental risk levels predicted by the proposed approach and the need for a better definition of these parameters.





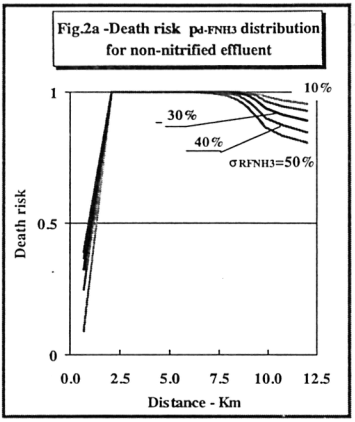


Fig.2a -Death risk $p_{d\text{-}FNH3}$ distribution for non-nitrified effluent
Death risk
1
0.5
0
10%
30%
40%
σRFNH3=50%
0.0 2.5 5.0 7.5 10.0 12.5
Distance - Km

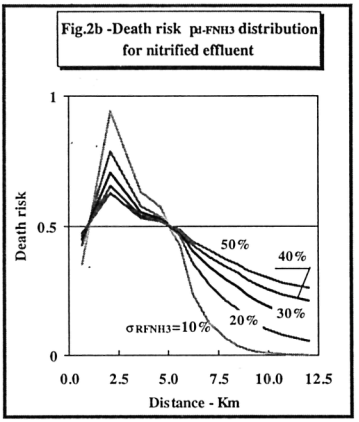


Fig.2b -Death risk $p_{d\text{-}FNH3}$ distribution for nitrified effluent
Death risk
1
0.5
0
50%
40%
30%
20%
σRFNH3=10%
0.0 2.5 5.0 7.5 10.0 12.5
Distance - Km

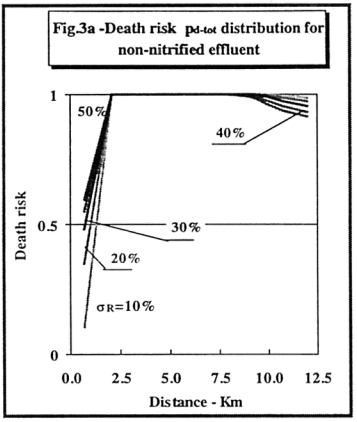


Fig.3a -Death risk $p_{d\text{-}tot}$ distribution for non-nitrified effluent
Death risk
1
0.5
0
50%
40%
30%
20%
σR=10%
0.0 2.5 5.0 7.5 10.0 12.5
Distance - Km

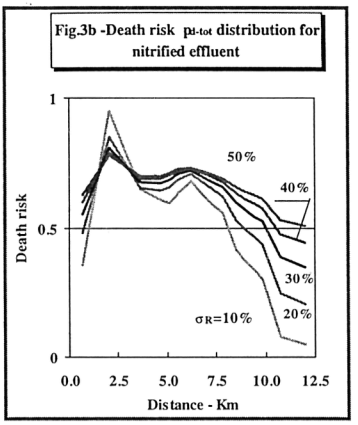


Fig.3b -Death risk $p_{d\text{-}tot}$ distribution for nitrified effluent
Death risk
1
0.5
0
50%
40%
30%
20%
σR=10%
0.0 2.5 5.0 7.5 10.0 12.5
Distance - Km

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PRACTICAL APPLICATIONS OF SENSITIVITY ANALYSIS IN ENVIRONMENTAL MODELING

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1 INTRODUCTION

Mathematical models, designed to simulate complex physical processes, are often used in scientific and engineering studies. For example, modeling the movement and consequence of radioactive pollutants is extremely important in the nuclear industry for environmental protection and facility control. One of the steps in model development is the determination of the parameters most influential on model results. A sensitivity analysis of these parameters is not only critical to model validation and uncertainty, but also guides future research.

The following is an assessment of several sensitivity analysis methods. It demonstrates calculational rigor and provides a comparison of parameter sensitivity rankings resulting from various sensitivity analysis techniques. The methods under comparison here have been summarized elsewhere [4]. An atmospheric tritium dosimetry model [3] is used as an example, but the techniques described can be applied to many different modeling problems.

2 SENSITIVITY ANALYSIS METHODS

The results of the application of ten sensitivity analysis techniques on an atmospheric tritium dose model [3] are presented. The sensitivity methods include the utilization of the following one-at-a-time sensitivity measures: partial derivatives (PD), one standard deviation increase and decrease of inputs (±SD), a 20% increase and decrease of inputs (±20%), and a sensitivity index (SI). The sensitivity measures investigated that utilize an array of input and output values generated through random sampling include: an importance index (II), a relative deviation of the output distribution (RD), a relative deviation ratio (RDR), partial rank correlation coefficients (PRCC), standardized regression coefficients (SRC), and rank regression coefficients (RRC). A Latin hypercube sampling procedure was used to generate an input array to the 21-parameter dose model with a sample size of 1000 [3].

In the dose model used here, parameter sensitivity is simplest to achieve by first aggregating the mathematical model, i.e., algebraically combining exposure pathway models, evaluating the resulting equation using best-estimate parameter values, and assessing the relative contribution to dose via each pathway component. Total atmospheric tritium dose to a downwind receptor is the sum of the inhalation and ingestion pathway doses and is given by,

$$D = \left\{\frac{4.84\text{x}10^{-9}\, T_e\, f_w\, C^a\, R_{pa}}{M\, H}\right\} \cdot \left\{ (2.74\, U_m\, f_m\, f_{pm}\, I_m\, e^{-(\lambda t_m)}) + (2.74\, U_b\, f_b\, f_{pb}\, I_b\, e^{-(\lambda t_b)}) + (1000\, U_v\, f_v) + (1000\, U_l\, f_l) + \left(\frac{(1.5)\, BR\, H}{f_w\, R_{pa}}\right) \right\} \quad (1)$$

where the constants account for unit conversions. Definitions of parameter distributions are given in Table 1. The five components in the right set of brackets represent the five exposure pathways: milk consumption, beef consumption, produce consumption, leafy vegetable consumption, and inhalation; respectively. It is immediately apparent that the model will be sensitive in some degree to three of the parameters in the left set of brackets (T_e, C^a, and M) since their values influence all pathway dose estimates. The three remaining parameters in the left brackets (f_w, R_{pa}, and H) cancel in the inhalation portion of the equation, therefore, they are expected to be sensitive parameters, but to have less influence than T_e, C^a, and M, since all pathway dose estimates are not affected by their values.

There are several statistical tests that involve some form of dividing or segmenting input parameters into two or more empirical distributions based on an associated partitioning of the output distribution [2]. In this example, for a given parameter, all input data associated with a dose below a specific partitioning point are said to belong to one random sample while input data associated with a dose above the same partitioning point belong to a second random sample. These two random samples are then used to generate the empirical distributions. Means, medians, variances, and other characteristics of these distributions are compared to determine whether the distributions are statistically identical.

Table 1. Parameter definitions and applicable exposure pathway models.

Description	Parameter
Average annual concentration of tritium	C^a
Effective biological half-life of tritium	T_e
Mass of soft tissue in adult male	M
Average annual absolute humidity	H
Percent water in vegetation	f_w
Ratio of plant to atmospheric tritium	R_{ja}
Consumption rate of milk	U_m
Fodder ingestion rate (milk cattle)	I_m
Feed-to-milk transfer factor	f_m
Fraction of fodder from pasture (milk cattle)	f_{pm}
Milk transport time (milking to consumption)	t_m
Consumption rate of beef	U_b
Fodder ingestion rate (beef cattle)	I_b
Feed-to-beef transfer factor	f_b
Fraction of fodder from pasture (beef cattle)	f_{pb}
Beef transport time (slaughter to consumption)	t_b
Consumption rate of produce	U_v
Fraction of produce from home garden	f_v
Consumption rate of leafy vegetables	U_l
Fraction of leafy vegetables from home garden	f_l
Annual average breathing rate of adult male	BR

Since their results are specific to the partitioning point, the sensitivity tests performed on the segmented data are not compared to the tests discussed above. The author has compared rankings for the Smirnov, Cramer-von Mises, Mann-Whitney, and Squared Ranks tests elsewhere [5].

3 RESULTS

Sensitivity results for each test have been obtained. Since one sensitivity method does not stand out as being universally accepted as the "correct" method, a "composite" sensitivity ranking has been determined. For the sake of comparing methods, the composite sensitivity ranking is based on the sum of ranks over all ten methods. The parameter with the lowest total rank is considered to have the greatest sensitivity. Iman and Conover [6] have presented a measure of "top-down correlation" for similar problems.

The relative performance of each method was determined by comparing the method-specific sensitivity ranking to the composite ranking. A "performance index" was calculated for this comparison. The performance index is a test of trend and is the sum of the squared-differences of the compared ranks, the T statistic in Spearman's ρ [1]. A smaller value for the index indicates a better trending of the method-specific and composite rank orders. The composite sensitivity ranking and the method performance ranking are shown in Table 2. Parameters are listed in decreasing order of sensitivity and the sensitivity techniques are listed in order of increasing performance index. Sensitivity ranks of the top ten parameters for each method are given in the table.

The test of trend using Spearman's ρ also was used to calculate a performance index and to compare sensitivity ranks between methods. These comparisons show which tests behave similarly and which tests appear to be inappropriate for sensitivity analysis, at least for the type of model considered in this work. Smaller values indicate better trending of ranks and greater parity between methods. As an example, the performance index for the comparison between the ±20% and PD methods is 1.5, indicating remarkable agreement between the two rank orders.

Table 2. Sensitivity ranking based on overall rank, listed in order of the composite ranking.

Parameter	SI	RD	RRC	±SD	PRCC	RDR	PD	±20%	SRC	II
Biological half-life	2	1	2	2	2	1	2	2	2	
Atmospheric concentration	1	2	1	1	1	2.5	2	2	5	
Produce consumption rate	3	3	3	3	3	9	8.5	8.5	1	2
Mass of soft tissue	4	4	4	4	4	2.5	2	2	7	
Plant/Atm HTO ratio	6	5	5	6	5.5	4	5	5.5	6	
Breathing rate	5	6	6	5	5.5	5	7	7	3	
Meat consumption rate	8	8	8	10	7.5				4	3
Leafy veg. consumption rate	7	7	7	9	7.5					4
Frac. Produce from garden	10	10	10	7		8	8.5	8.5	8	
Milk consumption rate	9								9.5	1
Feed-to-milk transfer factor		9			9	10				5
Absolute humidity						7	5	4		
Frac. from pasture (milk)										7
Percent water in vegetation						6	5	5.5		
Feed-to-meat transfer factor			9	8						6
Frac. leafy veg. from garden										
Beef cow ingestion rate										
Milk cow ingestion rate									9.5	
Frac. from pasture (beef)										8
Beef transport time										10
Milk transport time										9
Performance index	29	30	152	190	202	291	371	378	524	1404

4 DISCUSSION

As stated earlier, the performance of each method is measured by how closely the method-specific sensitivity rar compares to the composite rank. The performance index (PI) indicates that the SI and RD methods produce rankir results that are most similar to the composite rank (refer to Table 2). It is encouraging to see that all methods (exce the importance index) produce the same general ranking of parameter sensitivity. The importance index is meant to b used with simple additive or multiplicative models; it is apparently not appropriate as a sensitivity measure for tl model used in this example. The SI method chooses all of the top ten sensitive parameters while the RD methc chooses the top six parameters in the composite order. The first five methods choose the top six parameters, but n necessarily in the composite order.

A performance index was calculated for each combination of ten sensitivity techniques discussed to provide comparison between sensitivity methods. Small values of PI indicate similar sensitivity rankings. The parti derivative method is the most fundamental of the local sensitivity analysis techniques. It is appropriate only fi relatively small changes (on the order of several percent) in the input parameter. It is not surprising, therefore, th sensitivity ranks based on the PD and ±20% methods result in very similar orders. The standard deviation incremen (±SD) can at times be quite large, therefore, the ±SD ranks are not as similar. The RDR method acts globally, y produces rankings similar to PD and ±20%. As suggested by Table 2 and confirmed by the performance inde rankings obtained from the sensitivity index (SI) and the relative deviation (RD) are quite similar. And, to a less degree, the SI and RD methods produce results similar to the ±SD method. Parameter sensitivity ranks based on tl rank regression coefficient (RRC) are similar to the rankings from the SI, ±SD, and PRCC techniques. The importan index (II), meant for simple multiplicative models, produces results unlike any of the other methods; its utility questionable.

5 CONCLUSIONS

A number of sensitivity analysis techniques have been presented. The majority of the techniques result in similar rankings of the top several sensitive parameters. Since the actual ranking is not as important as the general ranking, most of the techniques would be appropriate for sensitivity analysis for the type of model considered in this report. The criterion most important, therefore, is the ease with which the sensitivity method can be performed. With the proper software, all methods presented here are relatively easy to execute. Given a moderate number of parameters and a hand calculator, however, the sensitivity index is the easiest and most reliable sensitivity measure. The SI can be calculated without detailed knowledge of the parameter distribution and without the use of random sampling schemes or large computer programs.

The relative deviation (RD) is a reliable measure of parameter sensitivity. Calculation of the RD is quite simple if a sampling technique is employed and the output values are stored for the statistical analysis. This analysis requires a one-at-a-time approach, however, and can be labor intensive. Estimating sensitivity based on the relative deviation ratio (RDR) is not recommended since its results are less reliable and it requires more calculational rigor than the RD.

Rank regression coefficients are easily obtained with the use of commercially available software. An electronic spreadsheet and the SAS statistical package were utilized for this analysis. The calculation of sensitivity rankings by varying the parameter over its standard deviation (±SD) is as simple as calculating the sensitivity index with the exception that some knowledge of the parameter distribution must be available. Varying the input parameter by a standard amount (±20%) is an easy test to perform, but its reliability is less desirable than the simpler SI method.

The simplest approach to conceptualize is the one-at-a-time method where sensitivity measures are determined by varying each parameter independently while all others are held constant. These sensitivity techniques, however, become rather time intensive with large numbers of parameters. The most fundamental of sensitivity techniques is the direct method of using partial differentials to calculate the rate of change in the model output with respect to a given input parameter. The one-at-a-time techniques are valid only for small variability in parameter values and the partials must be recalculated for each change in the base-case scenario.

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UNCERTAINTY AND SENSITIVITY ANALYSIS IN PERFORMANCE ASSESSMENT FOR THE WASTE ISOLATION PILOT PLANT

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The Waste Isolation Pilot Plant (WIPP) is under development by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic waste (TRU) [1, 2]. The WIPP is located in southeastern New Mexico, with waste disposal planned to take place in excavated chambers (i.e., waste panels) in a salt formation approximately 2000 ft below the land surface.

An important part of the development process for the WIPP has been a series of uncertainty and sensitivity analyses carried out by Sandia National Laboratories (SNL) to assess the current state of knowledge with respect to the WIPP and to provide guidance for future model development and research activities [3-6], with these analyses having been extensively reported in the journal literature [7-12]. The most recent uncertainty and sensitivity analyses [13, 14] have been carried out in support of an application by the DOE to the U.S. Environmental Protection Agency (EPA) for the certification of the WIPP for the disposal of TRU waste (i.e., the compliance certification application or CCA) [15]. If certified, the WIPP will be the first facility in the United States to begin operations for the geologic disposal of radioactive waste.

Regulations promulgated by the EPA (i.e., 40 CFR 191, Subpart B [16, 17]) determine the nature of the calculations carried by SNL to support the CCA and also the uncertainty and sensitivity analyses carried out as part of these calculations. The following is the central requirement of 40 CFR 191, Subpart B, and the primary determinant of the structure of the analysis (i.e., performance assessment or PA) carried out to support the CCA:

§ 191.13 Containment requirements.

(a) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based upon performance assessments, that cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall: (1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A); and (2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix A).

(b) Performance assessments need not provide complete assurance that the requirements of 191.13(a) will be met. Because of the long time period involved and the nature of the events and processes of interest, there will inevitably be substantial uncertainties in projecting disposal system performance. Proof of the future performance of a disposal system is not to be had in the ordinary sense of the word in situations that deal with much shorter time frames. Instead, what is required is a reasonable expectation, on the basis of the record before the implementing agency, that compliance with 191.13(a) will be achieved.

Containment Requirement 191.13(a) refers to "quantities calculated according to Table 1 (Appendix A)," which means a normalized radionuclide release to the accessible environment based on the type of waste being disposed of, the initial waste inventory, and the release that takes place (App. A, [16]). Table 1 (App. A) of [16] specifies allowable releases (i.e., release limits) for individual radionuclides. The WIPP is intended for TRU waste, which is

defined to be "waste containing more than 100 nanocuries of alpha-emitting transuranic isotopes, with half-lives greater than twenty years, per gram of waste" (p. 38084, [16]). Specifically, the normalized release R for transuranic waste is defined by

$$R = \sum_i \left(Q_i / L_i\right)\left(1 \times 10^6 \text{ Ci} / C\right), \tag{1}$$

where Q_i is the cumulative release of radionuclide i to the accessible environment during the 10,000-yr period following closure of the repository (Ci), L_i is the release limit (Ci) for the radionuclide i (Table 1, App. A, [16]) and C is the amount of TRU waste emplaced in the repository (Ci). For the 1996 WIPP PA (i.e., the PA carried out in support of the CCA), $C = 3.44 \times 10^6$ Ci [18].

To help clarify the intent of 40 CFR 191, the EPA also published 40 CFR 194 [19]. There, the following elaboration on the intent of 40 CFR 191.13 appears (pp. 5242-5243, [19]):

> § 194.34 Results of performance assessments.
>
> (a) The results of performance assessments shall be assembled into "complementary, cumulative distribution functions" (CCDFs) that represent the probability of exceeding various levels of cumulative release caused by all significant processes and events. (b) Probability distributions for uncertain disposal system parameter values used in performance assessments shall be developed and documented in any compliance application. (c) Computational techniques, which draw random samples from across the entire range of the probability distributions developed pursuant to paragraph (b) of this section, shall be used in generating CCDFs and shall be documented in any compliance application. (d) The number of CCDFs generated shall be large enough such that, at cumulative releases of 1 and 10, the maximum CCDF generated exceeds the 99th percentile of the population of CCDFs with at least a 0.95 probability. (e) Any compliance application shall display the full range of CCDFs generated. (f) Any compliance application shall provide information which demonstrates that there is at least a 95 percent level of statistical confidence that the mean of the population of CCDFs meets the containment requirements of § 191.13 of this chapter.

An interesting feature of analyses to assess compliance with 191.13(a), (b) is the requirement to incorporate two distinct treatments of uncertainty [20-22]. First, there is the uncertainty that leads to the CCDF specified in 191.13(a). This uncertainty results from an assumed randomness in what will occur at the WIPP site over the next 10,000 yr. Numerous designations for such uncertainty have been used in the literature, including stochastic, aleatory, variability, irreducible and type A. Second, there is the uncertainty characterized by the distributions called for in 194.34(b). This uncertainty results from a lack of knowledge about models and parameter values required in the construction of the CCDF specified in 191.13(a) and leads to the distribution of CCDFs called for in 194.34(c). Numerous designations for this characterization of uncertainty have also been used, including subjective, epistemic, state of knowledge, reducible and type B. In this presentation, stochastic and subjective will be used as the designations for these two types of uncertainty.

The terms uncertainty analysis and sensitivity analysis as used in PAs for the WIPP refer to assessments of the effects of subjective uncertainty. Specifically, uncertainty analysis designates an investigation of the uncertainty in model predictions that results from uncertainty in model inputs, and sensitivity analysis designates an investigation to determine the effects of individual variables on model predictions. Stochastic uncertainty enters into uncertainty and sensitivity analyses for the WIPP because the CCDF specified in 191.13(a), which derives from stochastic uncertainty, is the single most important result considered in such analyses.

Uncertainty and sensitivity analysis procedures used in the 1996 WIPP PA will be discussed and illustrated. Important topics to be covered include the use of Latin hypercube sampling [23] to propagate the effects of subjective uncertainty, the use of simple random sampling to propagate the effects of stochastic uncertainty, and the use of scatterplots, regression analysis, partial correlation analysis and rank transformations in sensitivity analysis to investigate the effects of subjective uncertainty [24].

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SOME BASIC RELATIONSHIPS FOR PARAMETER SENSIBILITY ANALYSIS IN STOCHASTIC ENVIRONMENT AND ITS APPLICATION TO THE DESIGN OF AN ADAPTIVE FILTER

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1 INTRODUCTION

When designing conventional algorithms for data assimilation in meteorology and oceanography one consiously or unconsiously assumes that the involved numerical model, in some sense, describes "well enough" a physical process under consideration and then one designs an algorithm based fully upon this numerical model. To deal with the problem of parametric model uncertainties (for instance, uncertainty in specification of the model error statistics), an adaptive filter (AF) is proposed in Hoang et al. (1994,1995) in which elements of the gain matrix are supposed to be estimated directly from observations by minimization of the prediction error. This approach is based essentially on some basic assumptions as unbiasedness of the model error, exact knowledge of model dynamics or on stationarity of the physical process which are, in many cases, incorrect. In fact, for example, the model error may be of nonstationary character which results in time-dependence of its statistics. Other sources of uncertainty are evidently the model bias and ill-specified model dynamics. It is well known that nonrobust behaviour of the filter may occur if there are large structure pertubations in the system description.

In this paper we present some preliminary theoretical and simulation results on an approach based on the theory of adjoints for detecting the changes in statistical properties of model error as well as system dynamics. Some basic relationships between variations of observed functionals and parameter pertubations in stochastic dynamics systems are obtained which reflect a sensitivity of these functionals with respect to changes in structures of parameters. Simulation for estimation of bias in model noise will be presented to show the difficulties of the problems and an effectiveness of the proposed approach.

2 SOME BASIC RELATIONSHIPS

The following stochastic system is an object of our study

$$x(t+1) = \Phi x(t) + b(t) + w(t), t = 0, 1, 2, ...N z(t+1) = Hx(t+1) + v(t+1), t = 0, 1, 2, ...N \qquad (1)$$

In (1) $\Phi \in R^{n \times n}$, $x(t) \in R^n$ is a true system state, $w(t)$ models the difference between the true physical system state and the numerical model. Thus $w(t)$ includes all errors, for example, error due to difference between the infinite full dimensional system and the actual system, error due to discretization, uncertainty in the boundary conditions, truncated physics ... We assume that $w(t)$ is a random process with zero mean and unknown covariance K_w. To avoid the situation when the model error has non-zero mean value, the vector $b(t) \in R^n$ is introduced which will be referred to as a bias of the model (1). In (1), $z \in R^p$ is an observation vector, $H \in R^{p \times n}$ is a known operator, $v(t)$ represents the measurement

error. We will assume that the matrix Φ and vector b may be a function of some unknown vector of parameters θ which may be a slowly time-varying vector-function.

2.1 Deterministic Case

(a) Full information case. First for simplicity let in (1), $w(t) = 0, v(t) = 0$ and $H = I$. It means that the state $x(t)$ is observed (full information case). Suppose that θ denotes the vector of unknown parameters in (1) (initial condition $x(0)$, some elements of Φ or b ...). Our task is : (i) to detect whether some guess θ^μ is far way from the true θ ? (ii) to generate an (optimal) estimate for θ.

Introduce the notation: $\langle x, y\rangle_n = \sum_{j=1}^{n} x(j)y(j)$, $x, y \in R^n, x(j)$ is the j^{th} component of x

Suppose that we are given (or we will construct) some functional of solution x of (1) subject to true value of θ (Marchuck, 1989)

$$J_\pi[z] = J_\pi[x] := \sum_{t=0}^{N} \langle \pi(t), x(t)\rangle_n \tag{2}$$

where $\pi(t) \in R^n$ doesn't depend on the true θ (but it may be a function of θ^μ). We want to use the functionals of the type (2) to infer on whether some value θ^μ is close to θ (since in practice θ is unknown). Let $\theta = \theta^\mu + \delta\theta$ and x^μ be the solution of (1) subject to θ^μ. Then for $J_\pi^\mu := J_\pi[x^\mu]$ let us compute $\delta J_\pi := J_\pi[z] - J_\pi[x^\mu]$. Introduce the following adjoint equation (AE) associeted with (1)

$$\phi^*(t) = \Phi^T \phi^*(t+1) + \pi(t), t = N, N-1, ...; \tag{3}$$

Then we have

Lemma 2.1

$$\begin{aligned} J_\pi[x] &= \langle \phi^*(0), x(0)\rangle_n + \sum_{t=0}^{N-1} \langle \phi^*(t), b(t)\rangle_n - \langle \phi^*(N+1), \Phi x(N)\rangle_n \\ &= J_b[\phi^*] + \langle \phi^*(0), x(0)\rangle_n - \langle \phi^*(N+1), x(N+1)\rangle_n \end{aligned} \tag{4}$$

Let us perturb θ by a small amount $\delta\theta$. Then from Eq. (1) $x(t)$ becomes $x(t) + \delta x(t)$ and approximately we obtain the following equation for the perturbed state δx

$$\delta x(t+1) = \Phi \delta x(t) + \delta\Phi x(t) + \delta b(t) \tag{5}$$

One sees that now $\delta J_\pi[z] = J_\pi[\delta x]$. Applying Lemma 2.1 to the functional $J_\pi[\delta x]$ where δx is the solution of (5), it is straightforward to show

Theorem 2.1. The following relationship holds for $J_\pi[\delta x]$

$$\delta J_\pi[x] = \langle \phi^*(0), \delta x(0)\rangle_n + \sum_{t=0}^{N-1} \langle \phi^*(t+1), \delta\Phi x(t)\rangle_n + \langle \phi^*(t+1), \delta b(t)\rangle_n - \langle \phi^*(N+1), \Phi \delta x(N)\rangle_n \tag{6}$$

Remark 2.1. Eq. (6) gives a relationship between $\delta J_\pi[x]$ and variations of all other parameters in the dynamical system (1) (initial and final state $x(0)$, $x(N)$, system dynamics Φ and forcing b ...). In general we are given a set of functionals of the type (2) and thus, a set of equations of the type (6), which allows us to infer on whether a particular value θ^μ is good enough to approximate θ and if necessary, to estimate the unknown $\delta\theta$. This technique is first proposed by Marchuck (1989) (presented in Hilbert space) for solving sensitivity problem in the inverse problems of mathematical physics.

Remark 2.2. For simplicity, one usually puts $\phi^*(N+1) = 0$. In addition, if the system (1) is stable and if we select $\pi(t) \neq 0$ only for large t then $\phi^*(0)$ will be very small (since Φ^T is stable). Initial state pertubation $\delta x(0)$ then doesn't influence on $J_\pi[\delta x]$ and it can be forgotten. As a consequence, we have

$$\delta J_\pi[x] = \sum_{t=t_0}^{N} \langle \phi^*(t), \delta\Phi x(t)\rangle_n + \langle \phi^*(t), \delta b(t)\rangle_n \tag{7}$$

where t_0 is a moment when $\phi^*(t), t \geq t_0$ are significant.

(b) Partial information case. Let us consider the general observation system (1). In fact now we can obtain from (1) only linear functionals of z, i.e. $J_\pi[z]$. To be able to apply the results in previous subsection, let us note that

$$\begin{aligned} J_\pi[z] &= \sum_{t=0}^{N}\langle \pi(t), z(t)\rangle_p = \sum_{t=0}^{N}\langle \pi(t), Hx(t)+v(t)\rangle_p \\ &= \sum_{t=0}^{N}\langle H^T\pi(t), x(t)\rangle_n + \sum_{t=0}^{N}\langle \pi(t), v(t)\rangle_p = J_{\pi'}[x]+\nu, \pi' := H^T\pi, \nu := J_\pi[v]. \end{aligned} \tag{8}$$

2.2 Stochastic case

Consider the situation when in (1) $w(t) \neq 0$. To be able to analyse a sensitivity of some observed functional with respect to unknown parameters in the model (1) in stochatic environment, let $\hat{z}^\mu(t/t-1) := \hat{z}(t/t-1;\theta^\mu)$ be some predictor for $z(t)$ conditioned by θ^μ. For an optimal in mean square predictor $\hat{z}(t/t-1;\theta) = H\hat{x}(t/t-1;\theta)$, $\hat{x}(t/t-1) = \Phi\hat{x}(t-1)$, the estimate $\hat{x}(t-1)$ is the solution of the Kalman filter (KF). Introduce a class of filters for the filtering problem (1)

$$\hat{x}(t+1) = L\hat{x}(t) + q, q := b + Kz(t+1), L := (I-KH)\Phi \tag{9}$$

Using this structure for $\hat{z}$ one can compute $J_\pi[\hat{z}(t/t-1;\theta^\mu)]$ hence

$$\delta J_\pi[z] := J_\pi[\hat{z}+\zeta] - J_\pi[\hat{z}^\mu] = J_\pi[\hat{z}] - J_\pi[\hat{z}^\mu] + J_\pi[\zeta] = J_{\pi'}[\delta\hat{x}] + \xi, \pi' := [H\Phi]^T\pi, \xi := J_\pi[\zeta] \tag{10}$$

Applying Theorem 2.1 to $J_{\pi'}[\delta\hat{x}]$ one obtains now the equation which relates $\delta J_\pi[z]$ to $\delta\hat{x}(0)$, δL, δq and $\delta\hat{x}(N)$

Theorem 2.2. Let $\hat{x}(t)$ be a solution of the filter (9). Then for $\delta J_\pi[z]$,

$$\delta J_\pi[z] = \langle \phi^*(0), \delta\hat{x}(0)\rangle_n - \langle \phi^*(N+1), L\delta\hat{x}(N)\rangle_n, \sum_{t=0}^{N}\langle \phi^*(t), \delta L\hat{x}(t)\rangle_n + \langle \phi^*(t), \delta q\rangle_n + \xi \tag{11}$$

where ϕ^* is the solution of the AE

$$\phi^*(t) = L^T\phi^*(t+1) + \pi'(t), \pi' := [H\Phi]^T\pi,\ t = N, N-1, \ldots \tag{12}$$

3 APPLICATION

This section presents application of Theorem 2.2 to the problem of estimation of bias in dynamical system. Suppose that the filter (9) is stable and only the vector b is unknown. Necessary condition for identification of b is $E[\zeta] = 0$. Let $\zeta^\mu := z - \hat{z}^\mu$. Then there is an interest to find $\hat{b}$ which yields $E[\zeta^\mu] = 0$. Remember that $J_\pi[\zeta^\mu] = J_\pi[z] - J_\pi[\hat{z}^\mu] = \delta J_\pi[z]$ hence, for example, for the choice $\pi(i) = (0, ..., 1/N, 0, ..., 0)^T$ where $1/N$ stands in i-th position, we have $J_{\pi(i)}[\zeta] \approx E[\zeta_i]$ where ζ_i is the i-th component of ζ. Evidently $\delta b = \hat{b} - b \neq 0$ implies $J_{\pi(i)}[\zeta] \neq 0$ hence one can use the value of $J_{\pi(i)}[\zeta]$ to estimate δb. Using some filter with fixed stabilizing gain K to produce $\hat{x}(t)$, from (11) follows $\delta L = 0$, $\delta q = \delta b$ and we have

Corollary 2.1. Let $\hat{x}(t)$ be a solution of a stable filter of the form (9). Let in (12) $\phi^*(N+1) = 0$. Then the following relations can serve as equations for determining δb : $\delta J_{\pi(i)}[z] = \sum_{t=1}^{N}\langle \phi_i^*(t), \delta b\rangle_n$, where ϕ_i^* is a solution of AE subject to $\pi = \pi(i)$, $i = 1, ..., p$.

4 CONCLUSION

We present some basic relationships between variation of observed functional and perturbations of parameters in stochastic dynamical systems. These relationships are useful for sensitivity analysis and parameter estimation. Some numerical examples will be presented for estimation of bias in a stable adaptibe filter. The question on the important role of function $\pi(t)$ will be also addressed.

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SENSITIVITY ANALYSIS FOR LONG-RUNNING COMPUTER-MODELS

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ABSTRACT

Sensitivity analysis is often performed in connection with uncertainty analysis. The affordable number of model runs is usually small for CPU-time intensive and thus long-running computer models. This has consequences for the type of uncertainty statements needed.
For efficiency reasons, sensitivity analysis has to use the runs performed for the purpose of uncertainty analysis. Since their number n is small and the number m of uncertainties is frequently large, correlation coefficients and standardized regression coefficients from stepwise regression (including ΔR^2 increase) are the only choice. Spurious correlation is inevitably present in the multivariate sample of size n and can often not be reduced or eliminated if m>n.
The correlation ratio is an indispensable sensitivity measure whenever model uncertainty is expressed by more than two model alternatives or when measures, quantifying degrees of linear or monotone realtionships, are not adequate. As a consequence of the small sample size n the correlation ratio is affordable only in approximate form.
Results from four actual analyses serve as examples. The experiences with these analyses also illustrate the outstanding role played by uncertainty and sensitivity analysis in the quality assurance of the computer model and of its application.

1 INTRODUCTION

Our primary goal is uncertainty analysis. We want to see the combined influence of all potentially important uncertainties on the model output. To this end, the state of knowledge with respect to phenomena, model formulations, model parameters, application-specific input parameters, controls of numerical solution algorithms, etc. is quantified and expressed by subjective probability distributions. Additionally, state of knowledge dependences, that might be influential, are suitably accounted for. As a consequence of these quantifications and of the logic encoded in the computer model, a subjective probability distribution results for each of the model output quantities. Quantitative uncertainty statements in the form of, for instance, 5% and 95% fractiles of these distributions could be immediately obtained if the distributions were known. In practice these fractiles have to be estimated from a random sample.

To this purpose we perform Monte Carlo simulation. We sample according to the specified marginal distributions and dependence quantifications of the uncertain quantities and perform a model run for each sample element (all uncertainties varied simultaneously). Since our models are CPU-time intensive (several hours or tens of hours on a modern processor) we can afford only small sample sizes, say $n \approx 100$. The n resulting values to each model output quantity constitute a random sample from the respective unknown subjective probability distribution and the desired fractiles can be estimated from this sample by standard statistical techniques.
Of course, if the resulting distributions are wide, which they often are, fractile estimates will be highly variable from sample to sample of size n. Therefore we need to quantify the possible impact of the sampling error. This is done by computing (u%,v%) statistical tolerance limits with, for instance, u=90 and v=95. They contain at least 90% of the combined influence of the quantified uncertainties at a confidence level of at least 95%.
Literature references for statistical tolerance limits, tables and approximate formulae can be found in [1]. The tables in [1] give the sample sizes needed such that the smallest or largest (resp. smallest and largest) model output value(s) in the sample are one-sided (resp. two-sided) (u%,v%) statistical tolerance limits. For example, 93 model runs are sufficient to have two-sided (95%,95%) statistical tolerance limits. These numbers depend only on the percentages u and v and are of course completely independent of the number of uncertainties taken into account.

Fractile estimates from a Latin Hypercube sample (LHS) can be expected to show less variability, yet statistical tolerance limits cannot be computed from an LHS and to simply provide the fractile estimates and claim that they are less variable than those from a simple random sample (SRS) does not suffice. Practical examples, even with n>100, have demonstrated this. The LHS estimates of the 95% fractile, for instance, can still be significantly below the true 95% fractile with no indication of how likely this shortcoming is. So we have to stick to SRS and tolerance limits.

Usually, the computer model is applied in order to provide input for some decision. Once the quantitative uncertainty statements are derived, the question arises whether the "best estimate" model output together with the quantitative uncertainty statement suggest that the intended decision can be meaningfully made. If the model output uncertainties are judged to be too large for the decision to be made we need to know where to primarily improve our state of knowledge. More precisely, do we have to give priority to further model development or is it specifics of the model application that we need to know better? To answer this question we perform sensitivity analysis.

Sensitivity measures from correlation and regression derived from an SRS of small size n may still exhibit considerable variability from sample to sample. This variability can be expected to be smaller in case of an LHS of the same size. However, because of what was said above this is no option for us. Also, we cannot have a separate sample for sensitvity analysis because of CPU-time (and calendar time) considerations. It is not only cost-effective (and in fact the only practically feasible way) but also natural and mathematically consistent, to exploit the same random sample used in uncertainty analysis for the purpose of sensitivity analysis.

In the next section we discuss the sensitivity measures that may be reasonably derived from small sample sizes in the presence of many uncertainties.

2 SENSITIVITY MEASURES ACTUALLY IN USE

The only measures suitable for small sample sizes are those from correlation and regression with and without transformation of parameter and model output values in the sample. Most frequently the probability integral or rank transformation is used. Since sample size n is small and the number m of uncertainties is often large we are bound to suffer from the influence of spurious correlations in our effort to compute sensitivity measures from correlation and regression. The matrix technique [2] to reduce spurious rank correlation in the sample is not applicable for m>n. This technique does not change the actual sample values but their combinations. It is not clear whether a simple random sample that was modified in this way can still be considered a simple random sample. A question that is of relevance with respect to the computation of statistical tolerance limits.

If all correlations $r_{j,k}$ ($j \neq k$; $j,k=1,...,m$) among the sample values $x_{i,j}$, $i=1,...,n$ were negligible, the square of the estimate of the standardized regression coefficient (SRC) of the regression of the model output Y on the uncertain parameter X_j , would be the fraction of the variability s_y^2 of the model output values y_i, explained by the variability s_j^2 of the parameter values $x_{i,j}$. Since the correlations $r_{j,k}$ are assumed negligible this interpretation also applies to the square of the estimate of the correlation coefficient (CC) $r_{y,j}$. Often, however, state of knowledge dependence between uncertain parameters is represented in the sample and, in the case of small sample sizes, spurious correlations are not negligible. In this situation the square of the estimate of the SRC is the fraction of the variability s_y^2 of the y_i , explained by that part of the variability s_j^2 of the $x_{i,j}$ that is not explained by the $x_{i,k}$, $k \neq j$, relative to the fraction of the variability s_j^2 of the $x_{i,j}$ that is not explained by the $x_{i,k}$, $k \neq j$.

The square of the estimate of the CC in this situation, however, still quantifies the fraction of the variability s_y^2 of the y_i, explained by the variability s_j^2 of the $x_{i,j}$. As a consequence of the simplicity of this interpretation, the CCs are more often used as sensitivity measures. They are also easier to compute than the SRCs. In the case of large numbers of uncertain parameters (m> n) SRCs for the main contributors to model output uncertainty would need to be obtained through stepwise regression.

Caution needs to be exercised in order to avoid misinterpretations. Reason is, that the CC to Y and X_j measures also the influence on Y of those uncertainty contributions which X_j has in common with X_k, $k \neq j$. This makes sense, but may lead to wrong conclusions about the influence of X_j and X_k on Y. Spurious correlations fake such common contributions.

lp to here "explained" meant "represented or captured by a linear function in one or more of the uncertain arameters". This restriction to a linear function may be unsatisfactory, i.e. it may be the cause for obtaining only an sufficient sample value of the square of the multiple correlation coefficient (or coefficient of determination) R^2.
o do away with this restriction, the so-called "correlation ratio" (CR) may be used as a sensitivity measure. The CR based on an approximation $y^{\sim} = h_j(x)$ of Y by a function of the uncertain parameter X_j alone. $h_j(x)$ does not need to e linear, nor is it required to specify $h_j(x)$ analytically and yet it is the best model of Y, as a function in X_j alone, in ie least squares sense.
he CR d_j is obtained from the relationship [3] $Var\{Y\} = E\{Var\{Y|X_j\}\} + Var\{E\{Y|X_j\}\}$ as
$^2 = Var\{E\{Y|X_j\}\} / Var\{Y\} = 1 - E\{Var\{Y|X_j\}\}/Var\{Y\}$. $E\{Var\{Y|X_j\}\}$ is a measure of the variability of Y ue to parameters other than X_j. It is zero if Y is a function of X_j alone. $Var\{E\{Y|X_j\}\}$ is the variability of the onditional mean value with respect to X_j. It is zero if Y is independent of X_j. In case Y is a linear function of the X_j, =1,...,m CR = CC.

Explained" stands here for "represented or captured by a function $h_j(x_{i,j})$ that provides the conditional mean value of at $x = x_{i,j}$". However, in the uncertainty/sensitivity analysis context all $x_{i,j}$ are random samples and there is zero robability for two or more identical sample values of X_j. Exceptions are model uncertainties, quantified by a small t of alternative model formulations; In other words: Parameters with only a small finite set of possibly applicable alues.

o obtain approximate CRs [4] the set of sample values $\{(x_{i,j}), i=1,...,n\}$ is divided into L disjoint classes with equally any (K) sample values in each class ($n = LK$). Then the class mean values are computed and $h_j(x_{i,j}) = E\{Y|X_j = x_{i,j}\}$ approximated by $h_j^{\sim}(x_{i,j}) = E\{Y|X_j$ from the class that contains $x_{i,j}\}$.

ince the CR measures the variability of conditional mean values, numbering and sequential order of the classes is relevant. This feature makes the CR the only sensitivity measure (of those discussed) suitable for model uncertainty uantified by a set of alternative model formulations. In this case model uncertainty is represented by an uncertain arameter with the finite number of indices of the model alternatives as alternative parameter values. Since indexing usually arbitrary, regression of Y on the parameter does generally not make sense.

^{2} small means, a least squares fitted linear regression model of Y in the X_j is not capable of explaining a major action of the variability s_y^2 of the model output values y_i, i=1,...,n. It follows: Neither SRC nor CC may be suited r ranking. What about the CR ? It will be suited, within the limitations of the approximate CR, since it is not stricted to a linear model. However, CR may be affected by outliers.

^{2} small will be due to strong nonlinearities of $Y=f(X_1,...,X_m)$. These may lead to extremal y_i values (outliers in the mple). All CR_j may be large due to few outliers. "Outliers" are often characteristic of strongly skewed subjective robability distributions of Y. In this case, fractions of s_y^2 explained may not be a suitable measure of the contribution f X_j to the uncertainty of Y since s_y^2 will be strongly affected by the outliers. A range, containing 90% subjective robability, may be a better expression of the uncertainty of Y, unless we are specifically interested in the outliers. herefore, measures operating on the cumulative probabilities of Y and the X_j may be more suitable for ranking. eason is, that one is not so much interested in an approximate model of the encoded relationship between Y and the j but rather in information about whether there are parameters X_j with a stronger tendency to give large y_i for large r small) $x_{i,j}$ than others. Therefore it will often suffice to look at the probability integral transformed values. As a onsequence, one investigates whether selection of an upper fractile of X_j will, in tendency, lead to an upper (or wer) fractile of Y, irrespective of the absolute values of Y and X_j involved, only differences in cumulative robability count.

his aims at statements about contributions to uncertainty as represented by the bulk of the population of values of Y nd not so much by extremal values. Sensitivity with respect to X_j is now ranked the higher the better the cumulative robabilities (or 1 - cumulative probability) of Y agree with those of X_j. Thus the bulk of the population of values of has a much higher weight in determining sensitivity than the extremal values which are relatively few in probability ontent (and thus in number in the sample). Unfortunately, the probability integral transform G_Y of Y is generally nknown. However, an empirical approximation is available from the sample values y_i. This is the rank ansformation of the y_i and of the $x_{i,j}$, j=1,...,m; i=1,...,n. From this approximation to the probability integral ansform standardized rank regression coefficients, rank correlation coefficients and correlation ratios on ranks are omputed, using $rk(y_i)$ and $rk(x_{i,j})$ instead of the probability integral transforms $G_Y(y_i)$ and $G_j(x_{i,j})$ j=1,...,m; i=1,...,n.

If the sample value of the square of the coefficient of determination after rank transformation $RR^2 > R^2$, the rank from rank transformed data is usually adopted. Be aware, that it ranks with respect to contribution to uncertainty expressed by the bulk of the y_i values and not so much by the extremal y_i since it is only difference in rank orders t counts and not absolute differences. What if RR^2 too is < 0.5? This leaves one with the rankings from CR and CF Studying scatter plots may help to clarify matters with respect to the question posed at the beginning, namely wh to improve the state of knowledge primarily.

3 PRACTICAL EXAMPLES

In the presentation of this paper the main points of the above section will be illustrated by results from four analy of computer model applications.

4 CONCLUSIONS

Sensitivity analysis is often performed in connection with uncertainty analysis and has to operate on the same mo runs for efficiency reasons.
Since uncertainty analysis for long-running computer models can only afford small numbers of runs, the uncertai statements have to be in the form of (u%,v%) statistical tolerance limits. These limits are only available from a sim random sample. As a consequence, sensitivity analysis has to use such a sample. Since numbers of uncertainties usually large and sample size is small spurious correlations play a non-negligible role but can often not be reduced eliminated if the number of uncertain parameters is larger than the sample size. The effect of spurious correlations sensitivity measures may be singled out by comparing CCs and SRCs.

The correlation ratio is an indispensible sensitivity measure where model uncertainties are expressed by more t two alternative model formulations and where measures quantifying degrees of linear or monotone relationship not adequate. As a consequence of the small sample size the correlation ratio is affordable only in its approxin form.

Access to a computing system with a sufficient number of parallel compute nodes, each capable of processing complete model, is definitely a strong asset in cutting back calendar time requirements of uncertainty and sensiti analyses of applications of long-running computer models.

Finally, the paramount importance of uncertainty and sensitivity analysis for the quality assurance of the compı model and its application must receive the strong emphasis which it so obviously deserves.

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EFFICIENCY OF DESIGNS FOR THE ANALYSIS OF VARIANCE OF MODEL OUTPUT

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1 INTRODUCTION

We study a scalar output Y of a deterministic model: $Y = f(X_1...X_k)$; in which $X_1...X_k$, are stochastically independent inputs or groups of inputs. The groups X_i may have different sizes. It will be assumed that Y has finite mean and variance. Then output Y can be decomposed into mean, main effects, and interactions up to order k:

$$Y = \mu + \Sigma_i \varepsilon_i + \Sigma_{i<j} \varepsilon_{ij} + \cdots \tag{1}$$

in which ε_i depends on X_i; ε_{ij} on X_i and X_j; etcetera [1,2]. The ε's have zero mean and variances σ^2_i, σ^2_{ij}, ...; they are uncorrelated but not independent. The variance is composed as:

$$\sigma^2_{tot} \equiv \mathrm{Var}[Y] = \Sigma_i \sigma^2_i + \Sigma_{i<j} \sigma^2_{ij} + \cdots \tag{2}$$

With respect to a group X_i, two variance components are particularly relevant. Firstly, MV[X_i], the *main effect variance* σ^2_i of X_i; and secondly IV[X_i], the *inclusive variance*: the sum of all variances σ^2 in the right-hand side of [2] in which subscript i is present. These two variance components are known under diverse names, from which we only mention the old *correlation ratio*: the main effect variance as fraction of the total variance [2,3,4,5,6]. Component MV[X_i] can be interpreted as the expected reduction in output variance when X_i would become known; and IV[X_i] as the expected variance that would remain as long as X_i would stay unknown [4]. Both variance components are of interest for the study of the composition of σ^2_{tot}.

Designs that allow the estimation of variances with a reasonable accuracy tend to be large. So there is a need to construct efficient designs [5,6]. The efficiency of a design to estimate these variance components depends on the model, the selected output and the distributions of the inputs. By that fact, general results are hard to obtain. In this paper we study the case that ε_i , ε_{ij} ... are independently normally distributed. This case can be studied with classical anova theory for random effect models. Although normality will not often arise in the uncertainty analysis of a model, it is hoped that the efficiency properties derived will be robust.

2 DESIGNS FOR TWO INDEPENDENT INPUT GROUPS

Denote the inputs under study by U and the complementary inputs by V; for instance, with k=5: $U=\{X_2,X_5\}$, and $V=\{X_1,X_3,X_4\}$. With some abuse of notation, we denote the model output studied by f(U,V).

The total variance σ^2_{tot} is equal to the sum of MV[U] and IV[V]. These three variances can be estimated without bias from a *nested* design that has an m×n data matrix

$$Y_{i,j}=f(U^{(i)}, V^{(i,j)}) \qquad (i=1...m;\ j=1...n) \tag{3}$$

We indicate independent draws from a random input by using different superscripts between round brackets. For instance, $V^{(1,1)}$, $V^{(1,2)}$ and $V^{(2,1)}$ denote independent draws of V. The design can be analyzed with standard anova. For maximal efficiency, the number of columns, n, should be equal to σ^2_{tot}/MV[U], rounded to an integer value [7]. A similar design, with U and V interchanged, allows estimation of MV[V] and IV[U]. Sobol' [2] proposed the following combination of two nested designs (with n=2) to estimate MV and IV of U and V :

$$Y_{i,1} = f(U^{(i,1)}, V^{(i,1)}) \qquad Y_{i,2} = f(U^{(i,1)}, V^{(i,2)}) \qquad Y_{i,3} = f(U^{(i,2)}, V^{(i,1)}). \tag{4}$$

Unbiased estimation of MV and IV of U and V is also possible with the following *alternating* des When going through its matrix in reading order, one encounters alternately new draws of U and V:

$$Y_{i,1} = f(U^{(i)}, V^{(i)}) \qquad Y_{i,2} = f(U^{(i)}, V^{(i+1)}) \qquad (i=1...m).$$

The total variance, σ^2_{tot}, can be estimated unbiasedly by the variance of either column. The inclusive variance is estimated without bias by the mean of the series $\frac{1}{2}(Y_{i,1} - Y_{i,2})^2$. Consecutive terms of this series are correl whereas terms further apart are independent. Thus, the variance of the mean of the series can be calculated standard time-series methods. Similarly, the inclusive variance of U is estimated by the mean of the series $\frac{1}{2}($ $Y_{i+1,1})^2$. The main effect variance MV[U] can be estimated as the complement of IV[V] with respect to σ^2_{tot}.

Obviously, unbiased estimation of MV and IV of U and V is possible with a *crossed* design, that ha data matrix

$$Y_{i,j} = f(U^{(i)}, V^{(j)}) \qquad (i=1...m;\ j=1...n).$$

For large m and n the crossed design soon becomes inefficient, because the interaction variance σ^2_{UV} is estim with much better accuracy than the main effect variances σ^2_U and σ^2_V. One should use replicated crossed de instead.

3 DESIGNS FOR MORE THAN TWO INDEPENDENT INPUT GROUPS

With increasing number k of input groups, replicated crossed designs, even at two levels per input, become inefficient. Sobol' designs for each input and are more promising [2,6].

A *winding stairs* design [4] allows estimation of MV and IV of all input groups considered. When g through the matrix of this design in reading order, one encounters cyclically new draws of $X_1, X_2 \ldots X_k$:

$$Y_{i,j} = f(X_1^{(i+\theta(j-1))}, X_2^{(i+\theta(j-2))}, \ldots, X_k^{(i+\theta(j-k))}) \qquad (i=1...m;\ j=1...k),$$

where $\theta(s)=1$ if $s \geq 0$ and $\theta(s)=0$ otherwise. Two columns of a winding stairs sample constitute an alternating d as treated above. Column 3 and 5, for instance, constitute an alternating design for $U=\{X_4, X_5\}$ and $V=\{X_6, X_1 \ldots X_3\}$. Thus, a winding stairs design allows estimation of MV and IV of all input groups X_i.

4 DISCUSSION

The designs mentioned permit unbiased estimation of the variance components under study. Moreove accuracy (variance) of the estimates can be estimated from the same designs, without assuming normality.

The Fourier Amplitude Sensitivity Test has not been treated, although it permits estimation of the variance components [6,8]. This design is of an altogether different type, since it applies only to independent s inputs. Furthermore, it is non-random, which demands other methods to assess accuracy.

Under assumption of normality, the accuracy of the estimators can be calculated analytically as fun of the variances to be estimated. The problem is that these variances are not known in advance. Thus possibility to extend designs according to results of intermediate analyses, constitutes an ingredient of effici Most designs mentioned can be extended in width and in length. In width, by starting with a sample of pc sources, and splitting only those pools that appear to be important. In length, by adding new replications appears that some estimates are not yet sufficiently accurate.

Efficiency is a clear concept when there is essentially only one estimand of interest, like in the case c nested design, where it was possible to pinpoint the optimal design. When the number of estimands is l however, it not easy to formulate an adequate optimality criterion. By this fact, it is hard to make ge statements about optimality.

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PARAMETERS OF CED SYSTEM MODELING NONEXPONENTIAL RELAXATION IN COMPLEX MATERIALS

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1 INTRODUCTION

In order to obtain an abstract stochastic description of relaxation phenomena in physical disordered materials [1] as well as of asset returns on financial markets [2] a class of CED systems in which the conditionally exponential dependence property can be attached to each element has been introduced [3]. The universal characteristics of the behavior of such systems are presented and disscussed according to the parameters.

2 DEFINITION OF CED SYSTEM

Independently of physical details complex condensed-matter systems (such as amorphous semiconductors, insulators, polymers, molecular solid solutions and glasses) have common properties. Namely, they consist of large number of random, strongly interacting species grouped in clusters and on the macroscopic level they exhibit universal characteristics in dynamical behaviour. In order to model relaxation phenomena in such systems we propose the stochastic description by the CED system.

Let $\{A_i, i = 1, 2, \ldots\}$ and $\{B_j^i, i, j = 1, 2, \ldots, j \neq i\}$ be two independent sequences of non-negative independent identically distributed random variables (r.v's). Let the constants $n \in \mathbf{N}$, $\tilde{b}_n$, r, $s > 0$, and $c \geq 0$.

DEFINITION.
A sequence $X_{1n}, \ldots X_{nn}$ of independent r.v's is called the CED system given $\{A_i, i = 1, 2, \ldots\}$ and $\{B_j^i, i, j = 1, 2, \ldots, j \neq i\}$ with the parameters $n \geq 2$, $\tilde{b}_n$, c, r, and s, iff it has the conditionally exponential dependence property, i.e., the conditional tails $P\left(X_{in} \geq x \,|\, A_i = a, \tilde{b}_n \max(B_j^i, j = 1, \ldots, n,\ j \neq i) = b\right)$ have for each $i = 1, \ldots n$ a common exponential decay form:

$$1 - G(x \mid a, b) \equiv \begin{cases} \exp(-ax^r) & \text{if} \quad c = 0, \\ \exp(-a \min(x^r, (b/c)^s)) & \text{if} \quad c > 0 \end{cases} \tag{1}$$

for a, b, $x \geq 0$. Sequences $\{A_i, i = 1, 2, \ldots\}$ and $\{B_j^i, i, j = 1, 2, \ldots, j \neq i\}$ can be interpreted as random input parameters while $X_{1n}, \ldots X_{nn}$ are output quantities of the model. In the CED system output data depend on input parameters according to exponential function (1).

3 ASYMPTOTIC BEHAVIOR OF CED SYSTEMS

Dynamical behavior of condensed-matter systems in the CED model is characterized by the following limit in distribution

$$\mathbf{X} = \lim_{n \to \infty} \tilde{m}_n \min(X_{1n}, \ldots, X_{nn}), \tag{2}$$

where $\tilde{m}_n, n = 2, 3, \ldots$, are positive normalizing constants. In Theorem 1 there are presented the conditions for input parameters of the system that guarantee the existence of the macroscopic output quantity **X**.

THEOREM 1.
Let the distribution function (d.f.) of r.v. B_2^1 is continuously differentiable. Assume that for sequences of positive constants $\{\tilde{b}_n, n = 2, 3, \ldots\}$ and $\{\tilde{m}_n, n = 2, 3, \ldots\}$ there exist the following non–zero limits in distribution:

$$\mathbf{A} = \lim_{n\to\infty} \frac{A_1 + \ldots + A_n}{\tilde{m}_n^r} \quad \text{and} \quad \mathbf{B} = \lim_{n\to\infty} \tilde{m}_n^{r/s} \tilde{b}_n \max(B_2^1, \ldots, B_n^1). \tag{3}$$

Additionally, let the limits **A** and **B** be finite with probability 1.

For any $c \geq 0$ there exists the nondegenerate limit in distribution (2) for a sequence $\{(X_{1n}, X_{2n}, ..., X_{nn}), 2, 3, ...\}$ of CED systems given $\{A_i, i = 1, 2, \ldots\}$ and $\{B_j^i, i, j = 1, 2, \ldots, j \neq i\}$ with the parameters n, $\tilde{b}_n$, r, s, and c. Moreover, the d.f. **F** of the limiting r.v. **X** has the form:

$$\mathbf{F}(x) = 1 - \exp\left(\int_0^x (1 - \mathbf{F}_B(cu^{r/s})) \frac{d}{du} \ln \mathcal{L}(\mathbf{F}_A; u^r) du\right)$$

where $\mathbf{F}_A$, $\mathbf{F}_B$ are the d.f.'s of the r.v.'s **A**, **B**, respectively. From the theory of stable distributions [4] and from the extreme value theory [5] it is known what are the only possible forms of the distributions of limiting r.v.'s in (3) and hence we obtain (in Theorem 2) that the r.v. **X** describing the dynamical behavior of the system can have only few possible probability distributions.

THEOREM 2.
Under the assumptions of Theorem 1:

- When $c = 0$ the limiting d.f. **F** obtains the form: $\mathbf{F}(x) = 1 - \exp(-(\Lambda_1 x^r)^\alpha)$.
- When $c > 0$ there are possible two types of the d.f. **F**:
  $\mathbf{F}(x) = 1 - \exp(-(\Lambda_1 \min(x^r, (b_0/c)^s))^\alpha)$
  and the solution of the following differential equation:

$$\frac{d\mathbf{F}}{dx}(x) = \alpha r \Lambda_1^\alpha x^{r\alpha - 1} \left(1 - \exp(-(\Lambda_2 c x^{r/s})^{-\gamma})\right) (1 - \mathbf{F}(x)), \ \mathbf{F}(0) = 0,$$

In all cases $x \geq 0$, $0 < \alpha \leq 1$, $\gamma > 0$
and Λ_1, Λ_2 are positive scale constants.

It is worth noting that to obtain above forms of **F** with $0 < \alpha < 1$ it is sufficient if

$$\lim_{a\to\infty} \frac{P(A_i > ax)}{P(A_i > a)} = x^{-\alpha} \qquad \text{for each } x > 0. \tag{4}$$

Moreover, to get third type of **F** it is sufficient if, additionally,

$$\lim_{b\to\infty} \frac{P(B_i^j > bx)}{P(B_i^j > b)} = x^{-\gamma} \qquad \text{for each } x > 0. \tag{5}$$

4 PROPERTIES OF THE PROBABILITY DISTRIBUTION OF X

Let us study now properties of the distribution function **F** in case $r = s = 1$, $c = 1$ and $(\Lambda_2)^\gamma = k(\Lambda_1)^\gamma$ for some $k > 0$ according to the parameters α and γ given by conditions (4) and (5). It appears that the behavior of the function **F** depends strongly on if $\gamma < \alpha$, $\gamma = \alpha$ or $\gamma > \alpha$ that is presented in the table.

Since the universality observed in the relaxation phenomena in physics, biology or economy has the form of two power law behavior, to explain this universality one can use CED systems satisfying conditions (4) and (5), however with $\gamma \geq \alpha$.

$\gamma < \alpha$	$\gamma = \alpha$	$\gamma > \alpha$
$\mathbf{F}(x) \underset{x\to\infty}{\longrightarrow} 1$ proper distribution		$\mathbf{F}(x) \underset{x\to\infty}{\longrightarrow} \mathbf{F}(\infty) < 1$ improper distribution
$\mathbf{F}'(x) \propto (\Lambda_1 x)^{-n}$ as $\Lambda_1 x << 1$		
	$\mathbf{F}'(x) \propto (\Lambda_1 x)^{-m-1}$ as $\Lambda_1 x >> 1$	
$n = 1 - \alpha$		
	$m = \alpha/k$	$m = \gamma - \alpha$
$0 < n < 1$ since $0 < \alpha < 1$		
	$m > 0$ since $k > 0, \alpha > 0$	$m > 0$ since $\gamma > \alpha, \alpha > 0$

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THE SENSITIVITY OF INDUCTION MOTOR NOISE LEVEL SCATTERING TO TECHNOLOGICAL PARAMETERS

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1 INTRODUCTION

For a last time the research workers and manufactures are concerned about acoustical noise generated by electrical machines. The reduction of acoustic noise of electric motors is one of the most attractive problem so far, and great efforts have been made for improvement.
A considerable variation in noise and vibration data among the members of a group of nominally identical mass-produced induction motors has been observed [1]. The performance of such motors to a considerable degree depends on the quality of the materials used in the construction and on the dimensional accuracy in production. The problem exist in securing a consistently high quality of produced machines. The scattering of parameters values of mass-produced motors, as a results of non-homogeneous quality of components, can be so large that some of the machines do not meet quality standards. Among the parameters of the low-power induction motors, where scattering happens to be particularly high, the noise level should be mentioned in the first place.

2 BASIS OF THE SENSITIVITY ANALYSIS METHOD

The parameters of electrical machines are functions of geometrical dimensions and physical properties of materials used in the constructions. Deviations of these quantities, to be subsequently called input quantities, depending on their interaction and statistical distribution, can in a different way influence the value of the end parameter. In mass production, which is a stochastic process, we may assume that all input quantities are independent and that their distribution is close to normal. In such a case the sensitivity to the variation of parameter $Y= f(X_1...X_i...X_n)$ of the variation of input parameters X_i can be written as:

$$(\gamma_Y)^2 = \sum_{i=1}^{n} (\alpha_i \gamma_i)^2 \qquad (1)$$

where:

- γ_Y - variation coefficient of parameter Y,. $\gamma_Y = \frac{\sigma_Y}{Y}$, σ_Y - standard deviation;
- γ_i - variation coefficient of input parameter X_i , $\gamma_i = \frac{\sigma_i}{X_i}$, σ_i - standard deviation;
- α_i - influence factor of input parameter X_i : $\alpha_i = \frac{\partial f(X_i...X_n)}{\partial X_i} \frac{X_i}{Y}$ (2)

Analysing equation (1) and (2), with known input quantity scatter parameters, one can determine the scattering of the end parameter Y and find the contribution of the individual input quantities to this scattering. The function describing the dependence (sensitivity) of a given parameter of an electrical machine on technological and constructional quantities has usually a very complex form and number of input quantities is considerable.

3 AN ALGORITHM FOR THE CALCULATION OF THE NOISE LEVEL OF SQUIRREL-CAGE INDUCTION MOTOR

Construction of the Algorithm

The mathematical model suggested for vibroacoustical effect in multi-pole three-phase squirrel-cage motors has been discussed in [2] and presented in [3]. The model has been expanded by phenomena bounded with harmonics of a stator current [4]. This led to the construction of an algorithm linking the level of noise in motors with technological and constructional quantities. Input data of the algorithm consist of about 100 quantities, together with their deviations. The algorithm includes (in given order) calculations of:
(a) mmf of elements of the magnetic circuit and of the magnetising current;

(b) stiffness of the shaft;
(c) clearances in bearings, bearing seats and bearing shield lock;
(d) static and dynamic eccentricity of the rotor;
(e) amplitude, frequency and the number of pole pairs of mmf air-gap harmonics, including saturation harmonics described by Frohne [6] and Yang [10], rotor harmonics and rotor residual harmonics following the method of Fruchtenich, Jordan and Seisch [5], generalised by Karkosinski [2];
(f) amplitude, frequency and the number of pole pairs of radial force waves on the internal surface of the stator bore;
(g) mass addition factor for longitudinal and rotational vibrations of teeth, ribs and of the stator winding after Frohne [6] and Yang [10];
(h) stiffness and damping factor of the base plate following the work of Frohne [6] and expanded by Karkosinski [2];
(i) amplitude of radial pulsating, unity-circumferential and circumferential mode vibration of the frame surface for harmonic components, taking into account reaction forces, following to the method of Jordan, Roeder and Weiss [7], generalised and expanded by Karkosinski [2];
(j) rms velocity of radial vibration of harmonic components, in 1/3 octave bands and total rms vibration velocity;
(k) relative sound intensity coefficient for harmonic components described by Jordan [8] and Yang [9, 10];
(l) A-weighted sound-power level of harmonic components and in 1/3 octave bands;
(m)A-weighted sound-power level.

Verification of the Algorithm

The degree, to which the algorithm represents real physical and technological relationship for sinusoidal supply, has been determined from the results of test on two types of squirrel-cage low-power motors (1.5 kW, number of poles 2p=4; 1.1 kW, number of poles 2p=6). This has been described in detail by Karkosinski [2, 3].
The test included:

- statistical measurements in the production process of anywhere from ten to twenty constructional quantities of motor components and complete motors,
- statistical measurements of vibration and noise level on two groups of one selected motor type for sinusoidal supply.

On the basis of measurement results, lists of input data for the algorithm were prepared and the calculations have been made. The total sound-power level for sinusoidal supply has been determined with an error not exceeding 6 dB(A). The additional calculations and laboratory measurements of the sound-power level for low-power induction motor fed by PWM current source inverter have been made. The total sound-power level inverter supply has been determined with an error not exceeding 8.5 dB(A).
Taking the above into account, it can be assumed that the applied flow chart of the calculation reflects relatively well the phenomena leading to the rise of noise of multi-pole induction motors where the aerodynamic noise is negligible.

4 EXAMPLE ANALYSIS OF NOISE LEVEL SCATTERING

Based on the algorithm for noise level calculations and by the use of the method of sensitivity analysis an algorithm for calculating the scattering of noise level was developed. In order to obtain formulas for partial influence factors, the algorithm functions were analytically differentiated by a computer.
Using the program to analyse the scattering of noise level calculations, detailed calculations were performed for a type of low-power mass-produced squirrel-cage motor designed for general purpose. Calculation results are presented in Table 1.

Table 1. Calculation results for the scattering of noise level for squirrel-cage 1.1 kW motors

Kind of the supply of motor	Upper limit of scatter range of sound power level (Value related to the mean value)
Sinusoidal supply 50 Hz	+ 5.1 dB(A)
PWM current inverter 50 Hz	+ 9.3 dB(A)

ıe results obtained of the computational analysis of scattering is the information of the contribution to it of ıividual input quantities. Table 2. lists the quantities, whose technological variations have the greatest influence the scattering of noise level. From almost a hundred input quantities only a few have a decisive contribution to ıttering of noise level. For sinusoidal supplied motor these are the dimensions of bearing node. The scattering of ise level can be limited by e.g. using higher-grade bearings. In case of current inverter-fed motor the scattering is used mainly by the tolerance of the stator dimensions.

Table 2. Analysis of the contribution to scattering of noise level for squirrel-cage 1.1 kW motors

Nr	Quantity with specified tolerance	Contribution to scattering	
		Sinus. supply	PWM inverter
1.	Diameter of bearing seat	27.7%	-
2.	Diameter of bearing ball	27.7%	-
3.	Diameter of outer bearing track	15.6%	-
4.	Diameter of inner bearing track	4.2%	-
5.	Radial run-out of rotor diameter	3.5%	-
6.	Stator bore (Int. diameter)	1.4%	7.8%
7.	External diameter of rotor core	-	8.2%
8.	Stator core length	-	32.7%
9.	Stator frame outer diameter	-	26.3%
10.	Stator cooling fin height	-	16.5%

CONCLUSIONS

ıe conclusion apply to the accuracy of the production process. The analysis of the scattering of the noise level of osen type of motors, gives directions concerning technological tolerance bands which are responsible for this atter. The motor production with reduced bands of external dimensions of the frame and the length of the stator eets leads to the reduced scattering of the noise level only in case of the current source inverter.
esented conclusions are an application example of the formulated algorithm and the prepared programs. By using ; proposed algorithm and applying sensitivity analysis it is possible to:

predict the level of noise within the total speed and load range for a given inverter topology and control strategy;

predict the level of noise and its scatter in case of design changes, introduction of new materials, changes in the technological process, and also in case of a newly-introduced series of machines;

minimise the scattering of the noise level of mass-produced motors by indicating quantities whose tolerance bands should undergo corrections;

improve the rationality of arrangement of inspection stations in production lines.

ıe method can be very useful for manufacturers for assessing the causes of excessive dispersion of vibration and ıise level of mass-produced motors, and for the designers of electrical drives. The method can also be applied to bration and noise data analysis of newly-designed machines.

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STATISTICAL THEORY ON DESIGN OF EXPERIMENTS, APPLIED TO SIMULATION

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1 OVERVIEW

This tutorial gives a survey on the use of statistical designs for what-if analysis in simulation, including (i) sensitivity analysis (SA), (ii) optimization, and (iii) validation/verification.

Sub (i): SA is divided into two phases. The first phase is a pilot stage, which consists of screening or searching for the important factors among (say) hundreds of potentially important factors. A novel screening technique is presented, namely sequential bifurcation. The second phase uses regression analysis to approximate the input/output transformation that is implied by the simulation model; the resulting regression model is also known as a metamodel or a response surface. Regression analysis gives better results when the simulation experiment is well designed, using either classical statistical designs (such as fractional factorials, including 2k - p) or optimal designs (such as pioneered by Fedorov, Kiefer, and Wolfowitz).

Sub (ii): To optimize the simulated system, the analysts may apply Response Surface Methodology (RSM); RSM combines regression analysis, statistical designs, and steepest-ascent hill-climbing.

Sub (iii): To validate a simulation model, again regression analysis and statistical designs may be applied.

Sub (i) through (iii): Several numerical examples and case-studies illustrate how statistical techniques can reduce the ad hoc character of simulation; that is, these statistical techniques can make simulation studies give more general results, in less time. For more details the readers are referred to [10].

2 WHY STATISTICAL DESIGNS?

'Design Of Experiments' or 'DOE' is a subdiscipline within mathematical statistics. This section addresses the questions: what is DOE, and why is DOE needed? These questions can be illustrated through the following two case studies.

The first case concerns an ecological study that uses a deterministic simulation model (consisting of a set of non-linear difference equations) with 281 parameters. The ecological experts are interested in the effects of these parameters on the response, namely, future carbon-dioxide or CO2 concentration; CO2 is the major cause of the greenhouse effect. The pilot phase of this study aims at screening: which factors among the many potentially important factors are really important? Recently, screening designs have been improved and new variations have been developed; details are given in [1] and [12].

The second case study concerns a Decision Support System (DSS) for production planning in a specific Dutch steel tube factory. The DSS and the factory are modeled through a stochastic, discrete-event simulation. The DSS is to be optimized. This DSS has fourteen input or decision variables; there are two response variables, namely, productive hours and lead time. Simulation of one combination of these fourteen inputs takes six hours of computer time, so searching for the optimal combination must be performed with care. Details are given in [8].

The following DOE terminology can be defined in a simulation context. A factor is a parameter, an input variable, or a module of a simulation model (or computer program). By definition, factors are changed during an experiment: they are not kept constant from run to run. Hence a factor takes at least two levels or 'values' during the experiment. The factor may be qualitative, for example, different priority rules corresponding with different computer modules. A detailed discussion of qualitative factors and various measurement scales is given in [7], pp. 138-142.

The central problem in DOE is the astronomically great number of combinations of factor levels. For example, in the ecological case study at least 2281 (> 1084) combinations may be distinguished. DOE can be defined as selecting the combinations of factor levels that will be actually simulated in an experiment with the simulation model. All designs are based on certain assumptions. It is possible indeed to investigate how to satisfy these assumptions 'Optimal' designs are yet of theoretical interest only [2]. After the selection of factor combinations to be run (the 'design'), the simulation

program is executed for these combinations. Next DOE analyzes the resulting input/output (I/O) data of the experiment, to derive conclusions about the importance of the factors. In simulation this is also known as what-if analysis: what happens if the analysts change parameters, input variables or modules of the simulation model? This question is closely related to sensitivity analysis, optimization, and validation/verification.

Unfortunately, the vast literature on simulation does not provide a standard definition of sensitivity analysis. We interpret sensitivity analysis as the systematic investigation of the reaction of the simulation responses to extreme values of the model's input or to drastic changes in the model's structure. For example, what happens when a parameter doubles; what happens if a module changes? So we do not focus on marginal changes or perturbations in the input values.

For this what-if analysis, DOE uses regression analysis, also known as Analysis Of Variance or ANOVA including Generalized Least Squares (GLS). This analysis is based on a metamodel or response surface, which is defined as a model of the underlying simulation model [4]. In other words, a metamodel is an approximation of the simulation program's I/O transformation. Typically, this regression metamodel belongs to one of the following three classes: (i) a first-order polynomial, which consists of main effects only, besides an overall or grand mean; (ii) a first-order polynomial augmented with interactions between pairs of factors (two-factor interactions); and (iii) a second-order polynomial, which also includes purely quadratic effects. The metamodel should be validated (not only the simulation model; see below): several lack of fit tests are available.

Most simulation models have multiple outputs, also called responses or criteria. In practice, multiple outputs are handled through the application of the techniques surveyed in this tutorial, per output type (see [6] and [7]). Optimization in the presence of multiple responses is also discussed in [8]. Optimization accounting for both the mean and the variance of the response is the focus of Taguchi's methods; see [13].

A metamodel treats the simulation model as a black box; that is, the simulation model's inputs and outputs are observed, and the factor effects in the metamodel are estimated. This approach has the following advantages and disadvantages.

An advantage is that DOE can be applied to all simulation models, either deterministic or stochastic, either in steady-state or in transient state. Further, DOE (including so-called `resolution-3' designs) gives better estimates of the factor effects than does the intuitive approach often followed in practice, namely the one-factor-at-a-time approach.

A disadvantage is that DOE cannot take advantage of the specific structure of a given simulation model, so it takes more simulation runs than do perturbation analysis and modern importance sampling, also known as likelihood ratio or score function. These alternative methods usually require a single run. Such a run, however, may be much longer than a run in DOE. Moreover, these alternatives require more mathematical sophistication, and they must satisfy more mathematical assumptions. (Importance sampling as a variance reduction technique -not a what-if technique- is important for rare event estimation, such as nuclear accidents and buffer overflows.) See [5] and [11].

DOE may be used not only for sensitivity analysis and optimization of simulation models, but also for their validation. The effect of data availability is then an important practical issue [9].

In summary, DOE is an important practical method for answering what-if questions in simulation. This is not surprising: by definition, simulation means that a model is used, not for mathematical analysis or numerical methods, but for experimentation. But experimentation requires a good design and a good analysis!

3 SIMULATION VERSUS REAL-LIFE EXPERIMENTS

DOE (with its concomitant regression analysis) is a standard topic in mathematical statistics and its applications to experiments with real-life (non-simulated) systems.. However, in simulation the). standard statistical techniques must be adapted such that they account for the following peculiarities of simulation.

(i) There are a great many factors in many practical simulation models. Indeed, the ecological case study (mentioned above) has 281 factors, whereas standard DOE assumes only up to (say) fifteen factors.

(ii) Stochastic simulation models use pseudorandom numbers, which means that the analysts have much more control over the noise in their experiments than the investigators have in standard statistical applications. For example, common and antithetic seeds may be used [7].

(iii) Randomization is of major concern in DOE outside simulation: assign the 'experimental units' (for example, patients) to the treatments (say, types of medication) in a random, non-systematic way so as to avoid bias (healthy patients receive medication of type 1 only). In simulation, however, this randomization problem disappears: pseudorandom number streams take over.

(iv) Outside simulation the application of blocking is an important technique to reduce systematic differences among experimental units; for example, tire wear differs among the four positions on the car: left front, ..., right rear. In simulation, however, complete control over the experiment eliminates the need for blocking. Yet, the blocking concept may be used to assign common and antithetic pseudorandom numbers [3].

4 CONCLUSIONS

(i) Screening may use a novel technique, namely Bettonvil-Kleijnen's sequential bifurcation, which is simple, efficient, and effective
(ii) Regression metamodeling generalizes the results of a simulation experiment with a small number of factors, since a regression metamodel estimates the I/O transformation specified by the underlying simulation model
(iii) Statistical designs give good estimators of main (first-order) effects, interactions between factors, and quadratic effects; these designs require fewer simulation runs than intuitive designs do
(iv) Optimization may use RSM, which combines regression analysis and statistical designs with steepest ascent; see (ii) and (iii)
(v) Validation may use regression analysis and statistical designs
(vi) These statistical techniques have already been applied many times in practical simulation studies, in many domains; these techniques make simulation studies give more general results, in less time.

All these issues are discussed in much more detail in [10], including nearly one hundred references.

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BOOTSTRAPPING AND CROSS-VALIDATION OF METAMODELS IN SIMULATION

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1 OVERVIEW

Bootstrapping is a resampling technique that requires less computer time than simulation does. Bootstrapping -like simulation- must be defined for each type of application. This presentation defines bootstrapping for random simulations with replicated runs. The focus is on linear regression metamodels or response surfaces. The metamodel's parameters are estimated through either Ordinary or Generalized Least Squares. Popular statistics for measuring the resulting fit of the estimated regression metamodels to the underlying simulation model are: (i) the coefficient of determination, denoted as R-square, (ii) R-square adjusted for the number of parameters, and (iii) the linear correlation coefficient, also known as Pearson's rho. This presentation proposes that the distributions of these three statistics be estimated through bootstrapping of the replicated simulation responses. A fourth statistic is Rao's lack-of-fit F-statistic. Bootstrapping of this statistic uses a different technique: the metamodel is fitted to the original, non-bootstrapped I/O simulation data, whereupon the estimated residuals are bootstrapped. A different approach is cross-validation, which may give Studentized prediction errors and which may use Bonferroni's inequality. There are several more validation statistics, such as the absolute relative errors, considering either their average or their maximum. These various fitting and validation procedures and different statistics are studied through an extensive Monte Carlo experiment. Queueing examples provide further illustrations of the practical use of these procedures and statistics.

2 DEFINITIONS: METAMODELS, CROSS-VALIDATION, AND BOOTSTRAPPING

A *metamodel* is an approximation of the input/output (I/O) transformation that is implied by a simulation model; the resulting black-box model is also known as a response surface. There are different types of metamodels. Examples are
(i) polynomial regression models, which are a type of linear regression;
(ii) splines, which partition the domain of applicability into subdomains and fit simple regression models to each of the subdomains;
(iii) neural networks, which are a type of non-linear regression.
Many references are given in [1].

Validation is defined by Sargent [2] as the 'substantiation that a model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model'. We shall assume that the simulation model itself - which is approximated by the metamodel - is valid. So we focus on the validity of the metamodel. First, the metamodel is 'fitted' (or 'calibrated') to a set of observations on the simulation model's I/O. Next the metamodel is 'validated' by predicting the outcomes of the simulation model for *new* factor combinations, and comparing these metamodel predictions with the corresponding simulation responses. Obviously, this definition of validation is very narrow; more general validation measures and procedures are discussed in [1].

In order to proceed proficiently, we define some symbols. We use Greek letters for parameters; capitals for matrixes; bold face for matrixes and vectors. We suppose that the simulation model has k factors, denoted by d_j with $j = 1, ..., k$ so $\boldsymbol{d} = (d_1, d_2, ...,d_k)$,. The symbol s_0 denotes the pseudo-random number seed, which plays a role only in *random simulation*. We assume a single type of response, denoted by w. Further, n denotes the total number of factor combinations actually simulated. In random simulation, factor combination i with $i = 1, ..., n$ may be replicated m_i times using non-overlapping pseudo-random number streams. This yields simulation response $w_{i;r}$ with $r = 1, .., m_i$. Hence, $N = \sum_{i=1}^{n} m_i$ denotes the total number of simulation observations. (Hence, $m_i = 1$ implies $N = n$.)

Cross-validation -more specifically, *leave-one-out cross-validation*- goes as follows:
(i) eliminate $(\boldsymbol{d}_i, w_{i;r})$, the I/O data of simulated input combination i;

(ii) re-estimate the metamodel from the remaining n - 1 combinations, assuming n - 1 observations suffice;
(iii) compute $\hat{y}_{-i}$, the forecast for combination i based on the metamodel in step (ii), and compare this forecast with the estimated expected simulation output $\overline{w}_i = \sum_{r=1}^{m_i} w_{i;r} / m_i$;
(iv) repeat this elimination for all values of i.

Note: Only if the metamodel as a whole is validated, it makes sense to study its individual parameters (say) β. Then it becomes interesting to observe how the estimated parameters change, as simulated factor combinations are deleted. Obviously, if the specified metamodel is a good approximation, then these estimates remain stable. Examples are given for polynomial regression metamodels in FMS (flexible manufacturing systems) and coal-transport studies in [3] and [4] respectively. In these metamodels the parameters can be interpreted as factor effects, so the metamodel can be used for explanation besides prediction. Other types of metamodels (e.g., splines, neural networks) are harder to interpret.

Bootstrapping is defined in the seminal book, Efron and Tibshirani ([5], p. 91), as follows (because we shall refer to this book frequently, we abbreviate it to E & T). The real world is described by $z \sim P$ where z is an independently and identically distributed (i.i.d.) variable (possibly, multi-variate), and P is its distribution function. Bootstrapping means that the data z_j ($j = 1, ..., s$) in the original sample of size s are randomly sampled with replacement. (Hence, each individual observation z_j may be sampled 0, 1, ..., s times; so this sampling follows a multinomial probability function). Let $\hat{F}$ denote the estimated probability function. Then the bootstrap sample is $z_j^* \sim \hat{F}$ where $\hat{F} = 1/s$ ($j = 1, ..., s$). E & T ([5], p. 115) comment that 'bootstrapping is not a uniquely defined concept'; and they continue (p. 383): 'alternative bootstrap methods may coexist'. We shall give different interpretations of bootstrapping for our problem.

Note: Bootstrapping is closely related to jackknifing; see E & T. Jackknifing was applied to Weighted Least Squares or WLS in [6]. Jackknifing is a linear approximation to bootstrapping. Many statistics in this paper, however, are not linear.

3 LITERATURE OVERVIEW

The *literature* gives the following picture. Stine [7] also examines bootstrapping in regression analysis, but he assumes that the regression model is correct (he focuses on prediction intervals and their coverage probabilities). Moreover he assumes constant response variances, whereas simulation applications show variance heterogeneity, in general. Breiman [8] investigates the selection of the correct regression model, but he assumes no replications ($m_i = 1$), constant response variances, and a particular parametric bootstrap of a particular statistic different from our's.

Bootstrapping in simulation raises an interesting question, not considered in E & T. Instead of using the computer to generate responses through bootstrapping, the computer may be used to generate more simulation responses, either for old factor combinations or for new combinations. In practice, many simulation models require much more computer time than regression analysis does. In those situations it makes sense indeed to bootstrap. Note that Breiman ([8], p. 750) also discusses bootstrapping versus replicating, but not in a simulation context.

4 OVERVIEW OF PRESENTATION

We *organize* the remainder of this presentation as follows.
(i) First we summarize linear regression metamodels. Their parameters are estimated through either Ordinary Least Squares (OLS) or Generalized Least Squares (GLS). Three popular statistics for measuring the resulting fit of the estimated regression metamodels to the simulation model are: R^2, the coefficient of determination, R^2_{adj}, the coefficient adjusted for the number of parameters, and ρ, Pearson's linear correlation coefficient.
(ii) The distributions of these three statistics are estimated through bootstrapping of the replicated simulation responses.
(iii) We summarize Rao's [9] lack-of-fit F-statistic for linear regression models. Basically, this statistic compares two variance estimators, namely one based on replications, and one based on residuals. The latter estimator is unbiased only if the metamodel is valid.
(iv) We bootstrap Rao's statistic, using the residuals of the metamodel fitted to the original, non-bootstrapped I/O simulation data. We also consider a parametric bootstrap that assumes Gaussian distributed simulation responses.
(v) We summarize cross-validation of linear regression metamodels. We studentize the prediction errors, that is, we divide these errors by their standard errors. Since there are n such errors, we take their maximum. To get a prespecified type-I error rate, we use Bonferroni's inequality.

(vi) We propose several other validation statistics, such as the absolute relative error. We take either their average or their maximum.
(viii) We propose an extensive Monte Carlo study that is taken from Kleijnen [10].
(ix) We propose queueing examples to illustrate the practical use of these statistics.
(x) We summarize the main conclusions.

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QUANTIFYING UNCERTAINTY IN MAPS OF TOXIC STRESS

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1 INTRODUCTION

The Potentially Affected Fraction (PAF) of species is a recently introduced indicator of toxic stress on ecosystems [1]. Basically, it gives the fraction of species exposed above their No Observed Effect Concentration (NOEC) (Figure 1). It is related to the Dutch system of setting environmental quality targets at a level where less than 5% of species is exposed above their NOEC. It has the advantage over similar dimensionless indicators such as concentration-to-target ratio that it is toxicologically meaningful, and can be compared between substances. A simple ratio is not suitable for this purpose, because the slopes of the effect curves may be different. Because the PAF is a fraction, we can simply combine the effects of two substances by:

$$PAF_{A+B} = 1 - (1 - PAF_A) * (1 - PAF_B) \quad (1)$$

This makes it particularly suitable to compare locations, which may have different mixtures of toxicants. More in general, the PAF can be used for mapping purposes which makes it a powerful tool for policy analysis, giving insight in such questions as "which sites should receive priority in remediation?" or "which areas are most sensitive to pollution?".

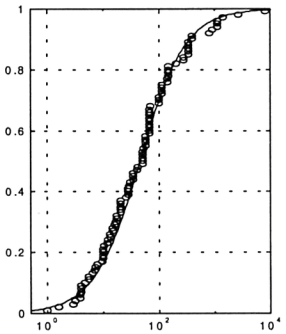

Figure 1 Cumulative distribution of NOEC's for cadmium in soil (left-hand panel). The fitted log-logistic curve can be used to derive quality objectives and the Potentially Affected Fraction of species (right-hand panel).

The calculation of the PAF involves considerable uncertainties at three levels:

- Environmental concentrations are generally poorly known, in particular if we are dealing with estimates by interpolation or modelling.

- Toxicity data are often scarce. The example of cadmium toxicity data in Figure 1 serves to illustrate the form of the NOEC-distribution, but the number of observations is not typical: often only three tests are available, making the estimated parameters of the cumulative distribution highly uncertain.
- Both field- and laboratory data on total contents of the toxicant should be corrected for biological availability. For soil organisms this implies estimating porewater concentration, which is the major exposure route.

As a result of these factors, maps of PAF have considerable uncertainties, which are of variable size for different toxicants. Another point of consideration is the non-Normality of the PAF distribution in combination with the nonlinearity of equation 1. As a result perturbation techniques do not give meaningful results. Monte Carlo techniques pose a considerable technical challenge because of the amount of data and the difficulty of characterising the resulting probability distributions.

This paper addresses the problem of taking uncertainty into account in combining maps of PAF of soil organisms for heavy metals and pesticides in The Netherlands. In this example, characterisation of uncertainty is important because much more is known about the group of heavy metals than about the pesticides. The results indicate the feasibility of quantifying uncertainty in the comparison between different environmental problems and the importance of uncertainty in drawing conclusions from such maps.

2 METHODS

Estimating environmental concentrations is the first step in mapping PAF. Maps of soil concentrations of heavy metals were interpolated from a large database (1000-2000 points, depending on the metal) taking into account both spatial variation and dependency on soil properties [2]. The resulting maps have a considerable local uncertainty, but in terms of overall statistical properties (mean, percentiles), the distribution of soil concentrations is well established. In contrast, there are no existing maps for pesticide concentrations. For the present study, maps of concentrations in non-agricultural soils of the 24 most important (in terms of use:toxicity ratio) pesticides were estimated on the basis of total use, volatilisation, atmospheric deposition and soil fate. Pesticide use is monitored for The Netherlands on a municipality level, for other European countries estimates were based on total use and landuse maps [1]. Volatilisation was estimated on the basis of chemical properties. Wet and dry deposition was calculated using a long-term averaged atmospheric model [3]. It turned out that the dominant uncertainty in this calculation was the volatilisation: different models gave more than an order of magnitude difference. In contrast, uncertainty about deposition rates have much less impact. Varying these results in a higher or lower degree of smoothing of the input map towards the output map. Because most pesticides are in widespread use in and around The Netherlands, this does not have a major effect on calculated total deposition. In view of the long calculation time required for the atmospheric model, uncertainty analysis was restricted to the volatilisation model only.

The toxicity of heavy metals to soil organisms is well known. Similar data as those presented in Figure 1 (cadmium) were available for copper, lead and zinc. Again, uncertainty about the toxicity of pesticides was much larger. For most pesticides, only acute toxic concentrations are known for three organisms only: an alga, a crustacean and a fish, making the resulting cumulative toxicity distribution highly uncertain. Moreover, the NOEC is based on chronic toxicity, which occurs at a lower concentration than acute poisoning. An estimate of this chronic/acute ratio could be based on a number of pesticides for which both acute and chronic toxicity were established , but uncertainty was considerable.

The calculation of porewater concentrations from total soil concentrations is relatively straightforward for pesticides, but less so for heavy metals. This is of particular concern as average field conditions are not identical to average laboratory conditions. The major difference is a pH value which is 2 points lower in the field, so that the calculations in fact require a considerable extrapolation.

The uncertainty in the calculations was quantified using a Monte Carlo sample. However, even using a sample of points on the map, the amount of data produced ([# of points] x [# of runs]) is too large to make an efficient overlay of maps (equation 1) feasible. For this reason, the resulting distributions were stored as quantiles of results. In order to overlay individual maps these quantiles were re-sampled in a new Monte Carlo run. The procedure is summarised in Figure 2.

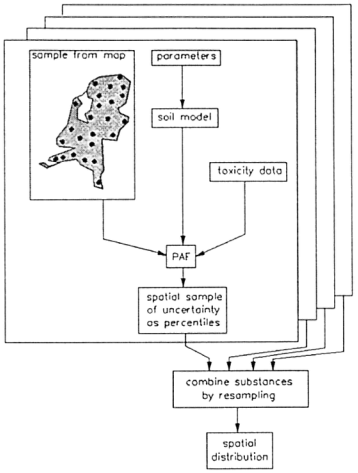

Figure 2 Procedure to generate uncertainty estimates of individual maps and of overlays.

3 RESULTS

Despite the fact that 24 pesticides were combined (which reduces relative uncertainty), the results for the pesticides are still considerably more uncertain than for the 4 metals (Figure 3). Quantifying this uncertainty is an important result in itself. As a best estimate, we might have concluded that pesticides generally pose much less of a problem than heavy metals. However, this gives only a partial answer. The question "is there a possible problem with pesticides?" should definitely be answered with yes. Instead of the obligatory remark that "more study is required" we are able to indicate the current range of uncertainty, allowing one to indicate the urgency of reduction of this range. In addition, quantifying uncertainty allows one to indicate areas of further research that require most attention.

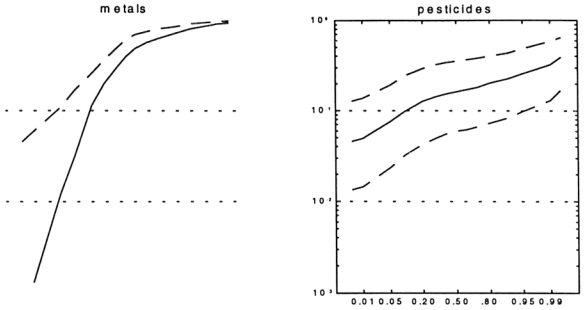

Figure 3 The combined PAFs for metals and pesticides as cumulative distributions of area. Graphs are given for median (drawn), 5th and 95th percentiles (dotted) of Monte Carlo results.

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STOCHASTIC SENSITIVITY ANALYSIS AND ADAPTIVE CRITIC REINFORCEMENT LEARNING

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1 INTRODUCTION

In this paper we study a stochastic implementation of reinforcement learning using the adaptive critic network architecture. In particular, we extend Koda and Okano's [1] Subconscious Noise Reaction (SNR) network to derive a new stochastic learning algorithm for the adaptive critic network. The adaptive critic architecture [2] is consisted of three components; i.e., plant, controller, and critic network. In the present study, the plant is assumed to be in the analytical form, and the control and critic to be parametric functions (i.e. neural networks). The plant is a model of reality which can be a network trained to emulate the system and its environment. The controller receives information on current state vectors x and outputs control vectors u. The critic network is placed hierarchically above other components which it advises, and monitors the trajectory of the plant and produces an output function J using the information on the control sequences.

In the implementation of adaptive critic reinforcement learning, a convenient parameterization may be through familiar sigmoidal neural networks, where the parameters are network weights. The critic network optimizes a scalar reinforcement signal J, which is used to advise the controller of the changes in its performance. Our goal now is to adapt the network weights w by transmitting the gradient (i.e. sensitivity) information through the critic to the plant and then to the controller. Thus, we can interpret this entire adaptive critic design as if the three components formed one large feedforward network. Hence, in the subsequent development, we treat the whole architecture as a single network, but our major focus be on the critic network.

The inputs at time t (hereafter, t denotes integer variables), are the vector of observables, $X(t)$. Let $J(t)$ be a scalar output of the critic network at time t which is an overall evaluation of how well the network is doing in creating a "good" situation. Then, in each time t, the controller is given a critical advice based on what kind of situation it produces: i.e., control actions $u(t)$ are "rewarded" if they lead to good results (larger $J(t+1)$) and "punished" if they lead to bad results (smaller $J(t+1)$). We assume that $J(t)$ is a function of the current input vector $X(t)$ and a set of network connection weights w, i.e., $J(X(t),w)$. We consider here the real-time learning where the network weights w are updated incrementally after each reinforcement signal is analyzed. Control and state vectors are then integrated into the plant model.

In the real-time formulation of utility optimization problem, there is only one target (reinforcement signal) because the network has single output $J(X(t),w)$. The training data at discrete time t is simply the input vector $X(t)$. Then, the target for time t, may be expressed as

$$J(X(t+1), w(t-1)) + U(X(t)) \tag{1}$$

where $w(t-1)$ is the old weight obtained at previous time $(t-1)$, and $U(X(t))$ denotes the utility function, which is a function of the current input vector $X(t)$, and plays the same role as a performance index or a cost function in optimal control theory [3].

In (1), $J(X(t+1),w(t-1))$ may be interpreted as a score to measure how good $X(t+1)$ is relative to the problem we started with -- e.g., maximizing the expected value of the utilities across all future times. For a typical utility maximization problem, we may write

$$J(X(t), w(t-1)) = \left\langle \sum_{k=0}^{\infty} \gamma^k U(X(t+k)) \right\rangle \tag{2}$$

where $\langle \cdot \rangle$ denotes the average or expected value and γ denotes the discount rate ($0<\gamma<1$) that accounts for uncertainty about future utilities which grows with time in the absence of reinforcement signal. We have assumed that the discounted sum in (2) converges.

Equation (1) implies that, before we begin the adaptation of network weight at time t, we use input vector $X(t+1)$ which may be an estimate of the input at (future) time $(t+1)$, and the old weight $w(t-1)$. The target function is then fixed for weight adaptation. In the weight adaptation phase, we modify the weight to try to reach the target. There are a number of supervised learning techniques to update the weights, and Werbos has shown that the heuristic dynamic programming (HDP) can be used for the reinforcement learning [4].

2 STOCHASTIC FORMULATION OF HEURISTIC DYNAMIC PROGRAMMING

In the formulation of HDP, we require knowledge of the utility function U, and the plant model which yields the current description of the system's behavior. The dynamic programming then produces a strategic utility function that is denoted by J^*. We may note that the function J defined by (2) can be viewed as an approximation to J^*. For our utility optimization problem, the key idea of dynamic programming [5] states that the maximization of the expected value of U over time, can be achieved by simply maximizing the J^* function in the immediate future.

As an explicit plant model for general (non-linear) noisy environment, we consider the following discrete-time stochastic system:

$$x(t+1) = F(x(t), u(t)) + \xi(t+1) \tag{3}$$

where $x(t)$ is the state vector, $u(t)$ is the control vector, and $\xi(t+1)$ denotes the Gaussian white noise with zero mean and unit variance. We interpret the stochastic difference equation (3) in the sense of Stratonovich and assume that there exists a stochastic neural network which represents the model (3). One should note that the Subconscious Noise Reaction (SNR) network may be used to obtain beneficial results from the ubiquitous noise term in (3) [1].

Through the plant model (3), both the critic and controller can exploit cause-and-effect information on the system states. It is important to note that we have used the state vector $x(t)$ in (3), since the states may usually be different from the vector of observables (inputs) $X(t)$. In general, states cannot be directly observable, but must be estimated from the past patterns or training data. However, it is natural to treat $X(t)$ as part of the state $x(t)$, since what we monitor is part of system reality. Accordingly, we may treat both U and J^* as functions of the system state, i.e., $U(x)$ and $J^*(x)$.

The function $J^*(x)$ can be found as a solution to the following modified form of Bellman equation:

$$J^*(x(t)) = \max\left\langle J^*(x(t+1))\right\rangle + U(x(t)) - U_0 = \max\left\langle J^*\left[F(x(t),u(t)) + \xi(t+1)\right]\right\rangle + U(x(t)) - U_0 \tag{4}$$

where we have used the plant model (3), and U_0 is the term used to prevent a possible divergence of the expected sum in (4). Under appropriate conditions, the existence of the optimal control can be shown such that $J(x)$ defined by (2) will converge to $J^*(x)$.

3 MAIN THEOREM

If we can directly estimate the derivatives of J^* with respect to the state vector $x(t)$, then the optimization of control sequence and weight adaptation may become an easy task. The partial derivative of J^* with respect to the state vector $x(t)$ constitutes a vector of sensitivity coefficients, $\lambda_i(t) = \partial J^*(x(t))/\partial x_i(t)$, which is equivalent to the familiar Lagrange multiplier or adjoint function used in the standard calculus of variations.

By direct differentiation of both sides of (4) with respect to $x_i(t)$, we obtain

$$\begin{aligned}\lambda_i(t) &= \max\left\langle \sum_j \frac{\partial J^*(x(t+1))}{\partial x_j(t+1)} \frac{\partial F_j(x(t),u(t))}{\partial x_i(t)} \right\rangle + \frac{\partial U(x(t))}{\partial x_i(t)} \\ &= \max\left\langle \sum_j \lambda_j(t+1) \frac{\partial F_j(x(t),u(t))}{\partial x_i(t)} \right\rangle + \frac{\partial U(x(t))}{\partial x_i(t)}\end{aligned} \tag{5}$$

where we have assumed that the operations of differentiation and expectation are interchangeable. Note that U_0 term in (4) has dropped. We may further note that $\lambda_i(t)$ can be computed directly from (5) by back-propagating sensitivities $\lambda_i(t+1) = \partial J^*(x(t+1))/\partial x_i(t+1)$. Thus, applying familiar back-propagation techniques and maximizing the expected sum in (5) across future time *(t+1)*, we can generate $\lambda(t)$.

We will now derive a new stochastic algorithm for the estimation of sensitivities of the strategic utility function J^* with respect to the state vector *x(t)*. For this purpose, we utilize the Novikov's identity $\langle H(\xi)\xi_i \rangle = \langle \delta H(\xi)/\delta \xi_i \rangle$: where $H(\xi)$ is an arbitrary functional of the Gaussian stochastic process $\xi(t)$, and $\delta H(\xi)/\delta \xi_i$ denotes the functional derivative [6][7][8]. Then, using the above identity, the following theorem is a straightforward result.

Theorem: For the plant model defined by (3), the following stochastic algorithm yields the computation of sensitivity coefficients:

$$\lambda_i(t) = \frac{1}{2}\max\left\langle J^*(x(t+1))\sum_j \xi_j(t+1)R_{ji}(x(t))\right\rangle + V_i(x(t)) \tag{6}$$

which is valid in a statistical sense (i.e., as a mean or average). In (6), we have defined, $R_{ji}(x(t)) = \partial F_j/\partial x_i(t)$, and $V_i(x(t))$ denotes the reinforcement function, $V_i(x(t)) = \partial U(x(t))/\partial x_i(t)$.

The detailed proof of the theorem is omitted here but note that the factor of *1/2* in (6) is derived from the definition of the equal time limit of the Stratonovich calculus.

4 SUBCONSCIOUS NOISE REACTION FOR REINFORCEMENT LEARNING

We can then extend the adaptive critic paradigm to the noise-based learning algorithm referred to as Subconscious Noise Reaction (SNR) (Koda and Okano [1]). Since we are considering the real-time learning, we can simply apply a single pass of SNR algorithm to update the weights using the gradient information obtained by applications of the main theorem. One should note that, unlike the error back-propagation, SNR does not require solutions to the equations of the back-propagation type but it directly updates the weights locally based on the ubiquitous noise. Hence, the present algorithm based on (6) has the potential for efficiently learning network weights with significantly fewer computations. The results may be a natural extension of the author's earlier results [6][7][8] to the adaptive critic reinforcement learning.

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ACYCLIC COMPARTMENTAL MODELS AND INFLUENCE DIAGRAMS

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1 INTRODUCTION

In this paper a method on determining a joint distribution on transfer coefficients in acyclic compartmental models is introduced. This method has been developed for the Joint CEC\USNRC Accident Consequence Code Uncertainty Analysis using Expert Judgment [1] and relates compartmental models with influence diagrams.

In doing uncertainty analysis a joint distribution on the *target variables*, the uncertain code input parameters, must be specified. An element of the methodology adopted in the joint project is to query the experts only on quantities which are physically observable, potential measurable and to which the expert can relate. Quantities for which the experts provide assessments are called *elicitation variables*. When target variables are unsuitable for elicitation the uncertainty analyst must determine a joint distribution on the target variables given the information on the elicitation variables. This task is known as Post-processing and is described in detail in [2] & [3].

The complexity of compartmental models encountered in the joint project is formidable. This necessitated the development of new techniques to enable tractable post-processing. Influence diagrams were found helpful in extracting conditional dependency structures embedded in compartmental models.

The main assumption linking compartmental models to influence diagrams is that functional independence entails statistical independence. This will be illustrated with an example.

2 EXAMPLE

CM-I (see Figure 1) is a very simple compartmental model which will be used only to illustrate the different steps which led to the new solution method.

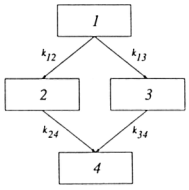

Figure 1: *CM-I*

For CM-I, the target variables are the transfer coefficients k_{ij} which describe the movement of radioactive material from box i to box j within a short time period. Based on Figure 1, a set of first order linear differential equations can be constructed which, with the appropriate initial conditions, fully specifies the movement of material between the compartments. Let $m_i(t)$ represent the amount of material in compartment i as a function of time t, furthermore let $\vec{k} = (k_{12}, \ldots, k_{34})$ and $F_{\vec{k}}$ be the

joint distribution on $\vec{k}$. The aim is to determine $F_{\vec{k}}$. Note that the uncertain quantities in Figure 1 are $m_1(t), \ldots, m_4(t)$ and $k_{12}, \ldots, k_{34}$. It was decided that the transfer coefficients were not suitable as elicitation variables; therefore the elicitation variables were on amount of material retained at different times in various compartments.

Like influence diagrams, acyclic compartmental model are directed acyclic graphs, but compartmental models aren't influence diagrams. For example, if a compartmental model were an influence diagram the following statement would be true ($\perp$ denotes statistical independence).

$$m_2(t) \perp m_3(t) \quad \text{given} \quad m_1(t) \tag{1}$$

Inspecting the equations derived from CM-I, however, it is easy to see that statement 1 is false. Briefly, the relevant equations for compartments $1, \ldots, 3$ are, starting at $t = 0$ with a unit deposit in compartment 1:

$$m_1(t) = e^{-(k_{12}+k_{13})\,t} \tag{2}$$

$$m_2(t) = k_{12}\,\frac{e^{-k_{24}\,t} - e^{-(k_{12}+k_{13})\,t}}{k_{12}+k_{13}-k_{24}} \tag{3}$$

$$m_3(t) = k_{13}\,\frac{e^{-k_{34}\,t} - e^{-(k_{12}+k_{13})\,t}}{k_{12}+k_{13}-k_{34}} \tag{4}$$

$m_1(t)$ gives information on $k_{12} + k_{13}$ only; from the equations of compartment 2 and 3 it follows that $m_2(t)$ and $m_3(t)$ cannot be considered statistically independent (any choice of k_{12} pins down k_{13}, because the sum $k_{12} + k_{13}$ is known). However, for fixed $t_0 > 0$ it follows from equations 7,...,4

$$\frac{m_2(t)}{m_2(t_0)} \perp \frac{m_3(t)}{m_3(t_0)} \quad \text{given} \quad k_{12}, k_{13} \tag{5}$$

Furthermore, given (k_{12}, k_{13}) we can express k_{24}, k_{34} in terms of $\frac{m_2(t)}{m_2(t_0)}$ and $\frac{m_3(t)}{m_3(t_0)}$, respectively. Hence it follows

$$k_{24} \perp k_{34} \quad \text{given} \quad k_{12}, k_{13} \tag{6}$$

Statement 6 lead to relating compartmental models and influence diagrams. The influence diagram of compartmental model CM-I is given in Figure 2

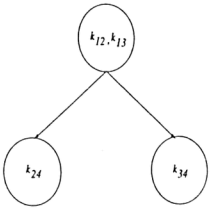

Figure 2: *The influence diagram of CM-I*

The influence diagram of CM-I can be used to infer conditional independence statements among the target variables $\vec{k}$. From Figure 2, it is easy to see conditional independence between (sets of) transfer coefficients. Using these conditional independence relationships $F_{\vec{k}}$ can be written as

$$F_{\vec{k}} = F_{k_{24}|k_{12},k_{13}}\, F_{k_{34}|k_{12},k_{13}}\, F_{k_{12},k_{13}} \tag{7}$$

3 SOLUTION SCHEME

The available data together with the insights gained from the influence diagram let to the following solution scheme

Step 1 Construct the influence diagram of CM-I

Step 2 Determination of the minimal information distribution $F_{k_{12},k_{13}}$ w.r.t uniform background measure.

Step 3 Determination of the minimal information distribution $F_{k_{24}|k_{12},k_{13}}$ w.r.t uniform background measure.

Step 4 Determination of the minimal information distribution $F_{k_{34}|k_{12},k_{13}}$ w.r.t uniform background measure.

Step 5 Combine the distribution obtained in Step 1,..., Step 4 using equation 7 to obtain $F_{\underline{k}}$.

The post-processing methods described in [2] & [3] will be used for the determination of the various distributions in Step 2, ..., Step 4.

Note that the 4-dimensional problem of Figure 1 is hereby reduced to two 3-dimensional problems, a 2-dimensional problem. A 13-dimensional problem will be discussed during the presentation and will be reduced to a number of distributions of lower dimension using the described technique.

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SENSITIVITY ANALYSIS IN A THRESHOLD SCENARIO. AN APPLICATION TO NUCLEAR CASES: REACTIVITY EXCURSIONS IN FISSION REACTORS AND IGNITION TEMPERATURE IN FUSION PLASMAS

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The performance of many natural mechanisms criticality depends on the value of a parameter, in relation to a threshold value. For instance, neutron chain reactions in a nuclear reactor are possible if and only if the reactivity is zero or positive [1]. Moreover, positive reactivity value induce exponential power evolution that can reach catastrophic effects, as happened in the Chernobyl accident [2].

Similarly, a self-sustained fusion burst can take place in a fusionable plasma if ignition conditions are achieved [3]. In the particular case of inertial confinement, the ignition onset can trigger a fusion burning wave across the compressed microcapsule [4]. Ignition requirements can be characterized by a threshold in the ion temperature of the plasma, once the isotopic composition and the rest of the plasma variables are given.

In both cases, fission and fusion, two approaches with different degree of complexity are used to analyze the behaviour of those mechanisms. The first approach is the *kinetic* one, which is based on the inmediate response of the system for some specified conditions. In the simplest form of the kinetic approach, it is only needed to know the value of the featuring parameter in order to determine whether the system will undergo a self-sustained evolution or will be quenched. In fission reactors, this parameter is the reactivity. In fusion plasmas, the ion temperature.

The second approach is the *dynamic* one, which takes into account the feedback mechanisms affecting the system evolution. In turn, this approach also has two levels of complexity: the linear dynamic model and the non-linear dynamic one [5]. In the former, the model equations are linearized around the working point, and it is valid for variables perturbations not exceeding 10% or so. In the latter, state variable can change without any limit, and the mechanical configuration of the system can suffer severe modifications. This was the case of the Chernobyl accident and will always be the case in Inertial Confinement Fusion microcapsules.

Although the physical mechanisms and governing equations of fission reactors and fusion plasmas are totally different, they show some common points for the analysis of the mathematical models describing those systems. First of all, they both are threshold scenarios. If the corresponding variable does not attain the threshold value, the system will not work. If the threshold is exceeded, the power evolution can be rather violent. In both cases, feedback mechanisms can help keep the evolution within acceptable values. This is what routinely happens in fission reactors and would happen in Magnetic Confinement Fusion devices. On the contrary, the evolution will be destructive in Inertial Confinement targets because the microcapsule is intended to explode.

The objective of this paper is to study the applications of sensitivity analysis to the dynamic behaviour of fission and fusion systems. The application is simple when the kinetic approach is used. Standard techniques can be applied to determine the sensitivity of the fission reactivity and the fusion ignition temperature to the main state variables [6]. The application is not so simple for the dynamic approach, because the proper description of the mechanical system and the feedback mechanisms is subject to large uncertainties.

For instance, in fission reactors the Doppler effect reaches saturation as the fuel temperatures approaches the melting point. Moreover, the temperature distribution in a reactor during an accident will not be uniform, and uncertainties in the temperature distribution must be taken into account in the feedback model, even if lumped parameters are used.

Another example can be presented on fusion plasmas. In a kinetic approach, ignition temperature is defined on the basis of the following criterion: The energy deposited in the fusion plasma by the fusion-born charged particles must overcome the radiation losses (in the same period of time). In general, it is considered that all the bremsstrahlung emission is lost (and this is the main component of the radiation losses).

In a more complex description, other feedback mechanisms must be taken into account. Both fusion-born neutrons and bremsstrahlung photons can deposit energy inside the plasma, and the deposition rate mainly depends on the areal mass of the plasma. When these mechanisms are embodied in the dynamic description of the system, the ignition temperature decreases. Uncertainties in the definition of the ignition temperature can be of importance in order to establish the requirements to produce energy from fusion reactions.

A main conclusion of our preliminary analysis is that physical implications of uncertainties are very different in fission reactors and fusion plasmas, when the system is close to the threshold. In fission reactors, the feedback mechanisms govern the system in such a way that a self-sustained neutron chain reaction is possible within a very broad domain of the state variables. In fusion reactions, (particularly in Inertial Fusion), there is not such a self-adjusting mechanism, and the threshold has to be tresspassed in order to make sure that ignition succeeds. In this case, uncertainties in the definition of the ignition temperature are directly transferred to the capability of burning the fusion fuel. If the ignition temperature can not be computed with a very high accuracy, and the calculated ignition temperature is lower than the actual ignition temperature, the fusion plasma will not iginite if it is heated just up to the calculated value.

On the contrary, a mistake in the calculation of the reactivity in a fission reactor does not hamper the possibility to establish a self-sustained chain reaction, if the reactivity error is not very big. Namely, if the error is much smaller than the fraction of delayed neutrons, criticality is established automatically because of reactor physics properties. State variables (fuel temperature and moderator density) adjust their values in a negative feedback cycle and reactivity is set to zero. For instance, in a typical Light Water Reactor, an error of $\pm$ 0.1% in reactivity can be compensated by a change in fuel tempreature of $\pm$ 50 ^{0}C.

These compensation mechanisms are nevertheless limited, and will not be effective if the threshold of prompt-criticality is exceeded.

Prompt-criticality corresponds to a reactivity value equal to the fraction of delayed neutrons. In this case, a second threshold appears, beyond which the exponential evolution of the neutron flux becomes much faster. Uncertainties both in the reactivity calculation and delayed-fraction estimates are very important in this case. Albeit the physical implications of the power evolution in a prompt-critical fission reactor and in a fusion microcapsule are very different, the mathematical model and the role of uncertainties are very similar. Sensitivity studies can help identify the main variables affecting the critical parameter of the system. In the case of a fission reactor, those variables have to be monitored in order to prevent a reactivity accident [1]. On the contrary, in fusion plasmas confined by inertial forces, the main variables have to be suitably enhanced in order to tresspass the threshold of ignition propagation. In the fission case, the most sensitive variable is the operating temperature of the fuel. In fusion plasmas, it is also the (ion) fuel temperature, although the areal mass is also of primary importance. Methods to reduce the uncertainties affecting these variables are therefore very useful to improve the accuracy of fission and fusion calculations.

In Inertial Fusion, uncertainties on the target performance arise from

1. target construction allowances
2. driver beam power history
3. beam energy deposition physics
4. hydrodynamic instabilities during the implosion phase
5. stoping-power of fusion born charged particles in a non-local thermal equilibrium plasma.
6. energy deposition in the plasma by fusion-born neutrons and bremsstrahlung.

Uncertainties from items 1 and 2 can be cut down by technology improvement. Points 3 and 4 present non-linear features, and some additional work is still needed to guarantee that the uncertainty level associated to them is minimized to acceptable values. Both experimental work and theoretical analysis can help reduce uncertainties stemming from points 5 and 6, which are the fundamental mechanisms to trigger ignition.

It is worth pointing out that two types of sensitivity analysis must be done in Inertial Fusion Research at the present level of knowledge:

- Sensitivity of the physical models used to interpret experiments and to make computational simulations.
- Sensitivity studies of the coefficients used in the model.

Physical models to characterize point 3,5 and 6 are still under discussion, because of the complexity of the mechanisms involved in them. In general, the physics of individual mechanisms is well-known, but there is a trend to elliminate some of them from the model, in order to make it more manageable. Sensitivity studies play here a very important role, because they can identify the actual significance of individual mechanisms and the loss in accuracy that can arise from neglecting each of those mechanisms. In relation to pint 3, beam energy deposition , the physical models obviously depend on the type of driver beam, with four main options

- laser beams
- heavy-ion beams
- light-ion beams
- cluster beam (molecular)

For instance, in the heavy-ion beam case, problems arising from range shortening due to higher temperatures are very important. Sensitivity studies based on deterministic codes using different characterization of ion-range shortering give very different results of the implosion history.

Similarly, laser-driven experiments of target implosions and foil acceleration are suitably simulated only in the case of introducing a tuneable parameter affecting the electron heat conduction. This parameter is the so called flux limiter, that must be around 0.03. Smaller or higher values significantly change the evolution of the target.

Another example of sensitivity analysis needed in the context of Inertial Fusion is the energy deposition by fusion-born neutrons. Early estimates of the physical consequences of this mechanism concluded that it was neglegible, but it was not so [7] when accurate calculations were carried out. As a matter of fact, contribution of neutrons to the reheating of fusionable plasmas are as high as that of alpha-particles in the case of targets with areal masses around or higher than 5 g/cm^2.

Sensitivity analysis on the coefficients characterizing thosc mechanisms are therefore of great significance. In relation to the former point, reducing uncertainties on the value of the kerma factors of the neutronic reactions of deuterium and tritium is an important objective.

Both deterministic computation codes and MonteCarlo calculations can be used in this extent. The main goal of sensitivity analysis is to identify the safety margin that is needed in a given design in order to guarantee that ignition (in fusion) is not going to be quenched because of the uncertainties associated to the governing mechanisms.

On the contrary, the safety margin in nuclear fission reactors must be understood as a reactivity margin that must not be tresspassed for not to reach prompt criticality (It is a true safety margin, in the strict sense of the word).

Sensitivity analysis are very important in both nuclear scenarios, fission and fusion, in order to improve quantitative accuracy, but the main conclusion drawn from the analysis is of a qualitative importance. Uncertainties in Nuclear Fission can be accomodated within the physics of the system when it is close to the criticality threshold, while uncertainties in Nuclear Fusion can not, if the errors make the ignition temperature tc lie below the actual threshold. Moreover, the highest importance of sensitivity analysis is in relation to the prompt-criticality threshold, where very strong power surges can happen. Uncertainties in the models and coefficients affecting this problem must be minimized, and a suitable safety margin must be identified in this case. thanks to sensitivity analysis.

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EVALUATING UNCERTAINTY IN STOCHASTIC SIMULATION MODELS

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1 BACKGROUND

This paper discusses fundamental concepts of uncertainty analysis relevant to both stochastic simulation models and deterministic models. A stochastic simulation model, called a simulation model, is a stochastic mathematical model that incorporates random numbers in the calculation of the model prediction. Queuing models are familiar simulation models in which random numbers are used for sampling interarrival and service times. Another example of simulation models is found in probabilistic risk assessments where atmospheric dispersion submodels are used to calculate movement of material. For these models, randomness comes not from the sampling of times but from the sampling of weather conditions, which are described by a frequency distribution of atmospheric variables like wind speed and direction as a function of height above ground. A common characteristic of simulation models is that single predictions, based on one interarrival time or one weather condition, for example, are not nearly as informative as the probability distribution of possible predictions induced by sampling the simulation variables like time and weather condition.

Simulation variability is an integral part of the simulation model, often corresponding to the stochastic variability one sees in the world or system being modeled. It is deliberately built into a simulation model. Simulation variability, however, is only one source of uncertainty in model prediction. There are two other major categories of uncertainty. One of these exists because models are based on assumptions which are usually selected with some latitude. The resulting source of uncertainty is called structural uncertainty, meaning that it is associated with the mathematical form or structure of the model. The other category of uncertainty is called input uncertainty, and refers to incomplete knowledge of "correct" values of model inputs, including model parameters. Input uncertainty exists independently of any model. For each specified simulation model, therefore, prediction uncertainty has two components, one from simulation variability and another from input uncertainty. Both components are relative to or conditional on the specified model. These components will be discussed in the sections that follow, but issues of structural uncertainty will not.

Distinguishing subjective input uncertainty and stochastic simulation variability is not new in model analysis. For example, Helton [1] identifies these sources of variation in probabilistic risk analyses for the U.S. Nuclear Regulatory Commission. In that paper, stochastic uncertainty—simulation variability—is captured by the complementary cumulative distribution function (CCDF), which is itself taken to be the model prediction. The CCDF is analyzed with respect to uncertainty and input importance. Apostolakis [2] uses the terms *epistemic* to refer to a knowledge related or subjective input uncertainty and *aleatory* to refer to stochastic simulation variability.

The language of model analysis is often general and vague, with terms having mostly intuitive meaning. The definitions and motivations for some of the commonly used terms and phrases offered in this paper lead to an analysis procedure based on prediction variance. In the following mathematical abstraction we present a setting for model analysis, relate practical objectives to mathematical terms, and show how two reasonable premises lead to a viable analysis strategy.

2 MATHEMATICAL ABSTRACTION

The principal notions discussed in this section are simulation variability, input uncertainty, prediction uncertainty, and importance of inputs. To set the stage, suppose that for a system model $m(\cdot)$, the prediction y is determined by two kinds of variables, denoted by the vectors x and z. The variables x are input variables in the deterministic sense. Inputs define initial conditions or state of a system being modeled and parameter values in the rules (equations and algorithms) that determine y from the initial conditions. The variables z are simulation variables.

They correspond to the random number streams used for the stochastic or random elements in rules which determine y in simulation models.

The model prediction is written as

$$y = m(x, z)\,, \tag{1}$$

where the vector z of simulation variables has a conditional probability distribution which depends on x,

$$z \sim f_{z|x}(z)\,. \tag{2}$$

For each fixed value x_0 of x, the prediction $y = m(x_0, z)$ is a random variable by virtue of the simulation variables z. We call the probability distribution of y as a function of x the *simulation distribution* of y, and write it as

$$y \sim f_{y|x}(y)\,, \tag{3}$$

meaning that it is a conditional probability distribution which depends on the value of x. The first two moments of the simulation distribution are called the *simulation mean* and *simulation variance*, denoted by $\mu_y^2(x)$ and $\sigma_y^2(x)$, respectively. Finally, uncertainty about proper or correct input values make it reasonable to treat the input vector x of length p as a random variable with probability distribution

$$x \sim f_x(x)\,,\ x \in D\,. \tag{4}$$

The *prediction distribution* is the unconditional (marginal) distribution of y, denoted by

$$y \sim f_y(y)\,. \tag{5}$$

The prediction distribution is induced by both the simulation variables z and the input variables x. The variance of the prediction distribution is called the *prediction variance*. In the limit, if the simulation distribution can be estimated with enough precision and accuracy that it is considered to be known without error, then the simulation distribution $f_{y|x}(y)$ itself (or, equivalently, the CCDF) might be studied as the output variable of a deterministic model, making consideration of the simulation variables z no longer necessary. Practically speaking, though, there is always *estimation error* associated with estimation of the simulation probability distribution.

We are now ready to consider objectives of the analysis. For the analyst, the objective of model analysis is to quantify uncertainty in y and to identify important components of the input vector x. For the decision maker, the objective is to discover and explore ways to control the real counterpart of the model prediction y. Thus, the terms "uncertainty" and "importance" need to be defined so that the analyst's objective corresponds to that of the decision maker. We begin with consideration of the notion of control.

The complication that simulation modeling introduces over deterministic modeling is that some uncertainty, namely, variability from simulation variables z, is intrinsic to the model. It is not possible to control simulation variability absolutely—reduce it to zero. On the other hand, the effect of input uncertainty might be diminished by allowable restriction of the value of the input vector x. More generally, though, we say that control of y—for the decision maker's objective—can be accomplished by changing the probability distribution f_x of the inputs x. In the decision maker's world, changing f_x would be accomplished by obtaining better information on x, in the case of both subjective probabilities and sampling distributions, or by effecting limitation on its value.

Particularly because x can be of high dimension, we phrase the objective of analysis as follows. The purpose of model analysis is to identify input subsets x^s whose joint probability distribution we consider for modification. The complementary subsets $x^{\bar{s}}$ will become random variables whose probability distribution is conditional on x^s. In the language of experimental design, the problem is to identify and determine the effectiveness of *control variables* x^s relative to *noise variables* $x^{\bar{s}}$. Consequently, we consider an alternative model prediction

$$\tilde{y} = E(y \mid x^s)\,. \tag{6}$$

We call $\tilde{y}$ the predictor of y based only on the control variables x^s, the values of the noise variables $x^{\bar{s}}$ and simulation variables z being averaged over. Therefore, the noise variables produce a prediction variability or uncertainty similar to that of the simulation variables z. The model prediction y, written in terms of x^s and $x^{\bar{s}}$, is

$$\begin{aligned} y &= \tilde{y} + (y - \tilde{y}) \\ &= E(y \mid x^s) + e(x^{\bar{s}}, z \mid x^s) \,. \end{aligned} \tag{7}$$

The first term represents the average fixed value we expect for y due to the control variables x^s. The second term represents the random residual or error component due to the variables $x^{\bar{s}}$ and z. The conditional expectation $\tilde{y}(x^s)$ is the usual regression predictor.

Assessment of the importance of the input subset x^s follows from two premises. First, the conditional expectation

$$\tilde{y} = E(y \mid x^s) \tag{8}$$

is the predictor based only on x^s of the full model prediction y. Second, the quality of $\tilde{y}$ as a predictor is measured by the quadratic loss function

$$\mathcal{L} = (y - \tilde{y})^2 \,. \tag{9}$$

The expected value $E(\mathcal{L})$ is commonly called the mean squared error (MSE) of prediction.

It is reasonable that the *importance* of the set x^s be related to its predictive ability, as measured locally by the loss function $\mathcal{L}$ and globally by the expected value of $\mathcal{L}$. Examining the global, mean squared error of prediction, we see that it is a function of the difference in variances given by

$$\begin{aligned} E(\mathcal{L}) &= E(y - \tilde{y})^2 \\ &= E(y - E[y \mid x^s])^2 \\ &= V(y) - V(E[y \mid x^s]) \\ &= V(y) - V(\tilde{y}) \end{aligned} \tag{10}$$

because

$$\begin{aligned} Cov(y, E[y \mid x^s]) &= \int y E[y \mid x^s] f_{x^{\bar{s}}, z \mid x^s} f_{x^s} \, dz \, dx^{\bar{s}} \, dx^s - \mu_y^2 \\ &= V(E[y \mid x^s]) \,. \end{aligned} \tag{11}$$

Using the well known variance formula from Parzen [3], we see that

$$\begin{aligned} V(y) &= V[E(y \mid x^s)] + E[V(y \mid x^s)] \\ &= V(\tilde{y}) + E(\mathcal{L}) \,. \end{aligned} \tag{12}$$

Hence, the correlation ratio of Pearson [4]

$$\eta^2 = V[E(y \mid x^s)] \,/\, V(y) \tag{13}$$

is a proper measure of the importance of x^s, and leads one to variance-based importance measures.

3 BEGINNING OF A STRATEGY FOR ANALYSIS

The last section argues that prediction variance can form a reasonable basis for analysis, a conclusion supported by the classical Analysis of Variance (ANOVA) analyses of statistics. Therefore, we consider an additive (linear) decomposition of the prediction variance $V(y)$ with terms that can be associated with the inputs x and simulation variables z. Writing

$$V(y) = V_1 + V_2 + \cdots \tag{14}$$

we suppose that the terms in the expansion represent contributions from subsets of inputs like, for example individual inputs, pairs or inputs, and so forth. Several ANOVA-like decompositions are available when the

components of the input vector x are statistically independent. They are presented by Cukier, Levine and Shuler [5], Efron and Stein [6], and Sobol' [7]. Cox [8] relaxes the independence requirement, but only somewhat. For the general case, which makes no assumptions about independence, Panjer [9] generalizes the well known variance formula as follows. Let $\{w_1, w_2, \cdots, w_k\}$ represent k random variables. Then, the variance of y can be written as

$$\begin{aligned} V(y) = & E_{w_k} E_{w_{k-1}} \cdots E_{w_3} E_{w_2} V_{w_1}(y \mid w_2, \cdots, w_k) \\ & + E_{w_k} E_{w_{k-1}} \cdots E_{w_3} V_{w_2} E_{w_1}(y \mid w_2, \cdots, w_k) \\ & + \cdots \\ & + V_{w_k} E_{w_{k-1}} \cdots E_{w_2} E_{w_1}(y \mid w_2, \cdots, w_k) \, . \end{aligned} \tag{15}$$

The terms in Panjer's formula can be individually associated with each of the w_j. However, because the random variables are not required to be statistically independent, the variance decomposition is not unique, but depends on the labeling of the set $\{w_1, w_2, \cdots, w_k\}$.

Panjer's formula can be used in analysis of simulation models as follows. For simulation variables z and the partition of the input vector x into x^s and $x^{\bar{s}}$, the prediction variance can be written as

$$V(y) = V_{x^s} E_{x^{\bar{s}}|x^s} E_{z|x}(y \mid x) + E_{x^s} V_{x^{\bar{s}}|x^s} E_{z|x}(y \mid x) + E_x V_{z|x}(y \mid x) \, , \tag{16}$$

where the subscripts of the operators indicate the variables of integration. The three terms, respectively, represent *nested* or hierarchical variance contributions from the control variables x^s, the noise variables $x^{\bar{s}}$, and simulation variables z. The number of such decompositions is the combinatorial function of the total number of inputs p and the size of the control variable subset and, therefore, may be enormous. Although the terms in Panjer's formula of Equation (16) are nonnegative, they are not variances, in general, unless the components of x and z are independent.

We interpret Equation (16) by noting that $E_{z|x}(y \mid x) = \mu_y(x)$ is the simulation mean of y, that the conditional expectation of the simulation mean over the noise variables $x^{\bar{s}}$ is the predictor $\tilde{y}$, and that the last term is the expected value of the simulation variance of y. Rewriting Equation (16) as

$$V(y) = V_{x^s}(\tilde{y}) + E_{x^s} V_{x^{\bar{s}}|x^s}[\mu_y(x)] + E_x\left[\sigma_y^2(x)\right] \tag{17}$$

shows how the prediction variance $V(y)$ arises from three sources: the control variables x^s, the noise variables $x^{\bar{s}}$ and the simulation variables z, as the three terms on the right side of Equation (17), respectively. We see, further, that the second and third terms on the right side of Equation (17) are themselves a decomposition of the residual variance $E(\mathcal{L})$ from Equation (12). Importantly, but at the cost of computer runs for estimation, the functional form of $\tilde{y}(x^s)$ is not assumed to be linear nor are the components of x^s and z assumed to be statistically independent.

4 REALITIES OF ESTIMATION

In theory, one can continue to extend the decomposition by expanding the second term on the right in Equation (17) to correspond to a partition of $x^{\bar{s}}$. Proceeding in this manner, one constructs a variance decomposition in the spirit of step-up regression, like in McKay and Beckman [10] and McKay [11]. A step-down procedure based on the simulation variance might prove more advantageous. Alternatively, best subset selection procedures might be developed. The relative sizes of (estimates of) terms would guide the development of the decomposition. In practice, however, good estimation of the components of the decomposition can become prohibitively time consuming, depending on the model $m(\cdot)$. Whatever direction one takes, important questions regarding estimation error and optimal sample designs remain to be answered.

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SENSITIVITY ANALYSIS FOR MODELING INCOMPLETE DATA

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1 INTRODUCTION

Missing data occur often and for a variety of reasons. In a repeated measures design it is common that some variables fail to be recorded for everybody. In longitudinal studies, missingness is often due to attrition. Many methods have become available to analyze incomplete data. Although most of the literature focuses on continuous outcomes, incomplete categorical data are also well studied. For categorical outcomes, incomplete data imply that a subject is not always classified into a single outcome category but rather into a set of categories, whereas the actual single category represents the complete data.

In this context, the terminology of Little and Rubin [8] is frequently used. The non-response process is said to be *missing completely at random* (MCAR) if the missingness is independent of both unobserved and observed data and *missing at random* (MAR) if, conditional on the observed data, the missingness is independent of the unobserved measurements. A process that is neither missing completely at random nor missing at random is termed *non-random*. In the context of likelihood inference, and when the parameters describing the measurement process are functionally independent of the parameters describing the missingness process, MCAR and MAR are *ignorable*, while a non-random process is non-ignorable. This terminology is based on the so-called *selection model framework* as opposed to the *pattern-mixture framework* (Molenberghs, Michiels, Kenward and Diggle [13]).

Recently, more modeling tools have become available for incomplete data, in particular with non-random dropout (see e.g., Diggle and Kenward [2], Kenward, Lesaffre and Molenberghs [6], Fitzmaurice, Molenberghs and Lipsitz [3], Goetghebeur and Molenberghs [4], Lesaffre, Molenberghs and Dewulf [7], Molenberghs, Kenward and Lesaffre [12], Michiels and Molenberghs [9], Molenberghs and Goetghebeur [10], Goetghebeur, Molenberghs and Katz [5]). These methods find their way into the broad statistical community. Less widespread is the awareness of computational and interpretational problems that arise when such methods are used without extreme caution. Indeed, one should be aware of possible occurrence of boundary and invalid solutions, as well as non-unique solutions to the maximum likelihood equations. Examples of this problem are found in Little and Rubin [8] (Section 11.6), Baker and Laird [1], Park and Brown [15], and Molenberghs, Goetghebeur and Lipsitz [11].

2 THE NEED FOR SENSITIVITY ANALYSIS

¿From this work emerges the awareness that models often yield the same or similar fits to the *incomplete observed data*, but produce qualitatively different predictions for the unobserved data. One should be

aware of the potential danger of unidentified (sets of) parameters, i.e. for which the data provide no information. Even if the degrees of freedom are not saturated, the MLE may be obtained on an entire subset of the parameter space. Scanning a range of values for one or more parameters and maximizing over the remaining ones can yield an enlightening sensitivity analysis. In the absence of a point estimate, some conclusions can be drawn from these ranges. Scanning the entire range can be seen as a sensitivity analysis. This route has been explored before by Nordheim [14], where a model is reparameterized such that a sensitivity analysis can be conducted in terms of a meaningful parameter.

Even when the model under consideration is identifiable, this is invariably based on strong models assumptions. Hence, also here there is a clear need for analyzing the sensitivity of the inferential procedures used to these assumptions. We will discuss both informal and informal routes for sensitivity analysis.

In real applications, contextual information can help discriminate between models that are not distinguishable on purely statistical grounds. We stress the importance of using all available additional information, including prior knowledge (to determine the more plausible models), the temporal and/or association structure among repeated measures, and covariate information to extend the range of plausible models (in particular if a reason for dropout or missingness has been recorded, as is often the case in clinical trials). In the same example, several plausible models yield the same qualitative conclusions.

3 UNCERTAINTY, IMPRECISION AND IGNORANCE

More formally, we will introduce the distinction between two sources of *uncertainty*: *imprecision* and *ignorance*. Imprecision stems from the fact that inferences are drawn from a finite sample thought representative for a larger entity (e.g., a population). It shrinks and vanishes when the sample size tends to infinity. Ignorance stems from the fact that a part of the data is missing (e.g., 25% of the trial subjects have only one out of two designed measurements). Imprecision is quantified in standard statistical theory by means of such measures as standard errors or confidence intervals (or confidence regions). The well-developed statistical theory has made the quantification of imprecision routine practice. Ignorance is not established as a formal concept and arguably this is the cause for the lack of (formal) sensitivity analyses in the context of incomplete data. Therefore, it is necessary to supplement the existing toolkit with *intervals of ignorance* (or regions of ignorance) and combine both measures into a *more honest* quantification of uncertainty.

4 ILLUSTRATION

These concepts are illustrated using contingency tables. As a simple but illustrative example, consider a binary random variables on which r successes are scored, $n - r$ failures, while $N - n$ subjects fail to respond. When the odds for success is of interest, the missing (completely) at random estimate is $\hat{\eta} = 3Dr/(n - r)$, while the corresponding interval of ignorance is $\hat{\eta}_\lambda = 3D\lambda r/(n - r)$, with

$$\frac{n - r}{N - r} \leq \lambda \leq \frac{N - (n - r)}{r}.$$

Obviously, $\lambda = 3D1$ corresponds to MCAR, while all other values indicate a particular informative model. Indeed, the probability of being observed is assumed to be q when the true measurement is success, while it is λq when the true measurement is failure, and both probabilities are equal when $\lambda = 3D1$. A graphical method to display the interval of ignorance, together with the interval of uncertainty, and the confidence intervals for each λ, will be discussed. Alternative approaches will be discussed, as well as more complex settings. Tools to assess the *validity* of the approach, analogous to, e.g., coverage of confidence intervals, will be presented.

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SENSITIVITY ANALYSIS ON A CROP GROWTH MONITORING SYSTEM

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The MARS Project from the Space Applications Institute of the Joint Research Centre has been set up to provide the EC (DG VI - Agriculture) with objective, homogeneous and timely information on agricultural production of the E.U. Member States. To achieve this goal, remote sensing, geographic information system and agrometeorological modelling techniques have been combined to provide agricultural production estimates at European level.

1 INTRODUCTION TO THE MODEL

Quantitative crop yield information is obtained by agrometeorological modelling to simulate the growth of crops throughout the agricultural season. The Crop Growth Monitoring System (CGMS) is driven by meteorological conditions, modified by other environmental factors. This mechanistic approach explains crop growth on the basis of underlying processes, such as photosynthesis and respiration. The model uses a combined energy balance / water balance module which compares real transpiration with calculated potential transpiration. It describes the crop life cycle from sowing to maturity on a daily time step. Crop growth is simulated (i.e. leaf area index, biomass, storage organ accumulation) in combination with phenological development.

CGMS is made of sub-systems which are run sequentially [1] :

- Weather monitoring. This module processes daily meteorological data into inputs required by CGMS (rainfall, temperature, radiation, evapotranspiration). Meteorological inputs are interpolated from weather stations on grid-cells of 50x50 kms.
- Crop growth monitoring. Simulations are performed on a daily basis to provide quantitative indicators of crop growth using (i) the interpolated meteo parameters on grid-cells, (ii) soil characteristics and (iii) region specific crop parameters.

2 DATA DESCRIPTION

2.1 Input data.

- Average meteorological data, cumulated from crop emergence to maturity. Historical mean over 20 years for temperature (^{o}C/day), global radiation (J/m^2), potential evapotranspiration (mm) and rainfall (mm).
- Soil characteristics, described by its depth (Table 1) and its water retention capacity (Table 2).
- Crop parameters, in term of required sum of temperature for a given variety of a given crop to complete its full development cycle from emergence to maturity (Table 3). Wheat being the main culture in Europe, the analysis will concentrate on this crop.

While meteorological variables are quantitative, soil parameters and varieties are categorical.

Table 1: Soil Rooting Depth

RD	Soil Depth (cm)
1	0 to 10
2	10 to 60
3	60 to 80
4	80 to 100
5	100 to 120

Table 2:Soil Physical Group

SPG	Water Capacity Retention (cm of water per m of soil)
1	14
2	17
3	20
4	23

Table 3:CGMS variety for wheat

Var	Sum of temperature (°C/d) emergence→maturity
1	2000
2	2050
3	2150
4	2200
5	2250
6	2300
7	2350

2.2 Data exploration

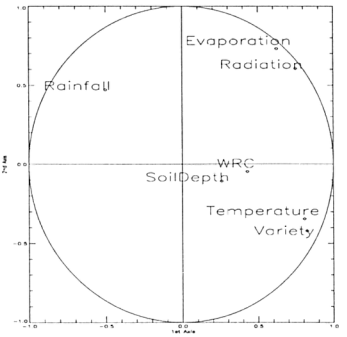

Figure 1: Correlation circle of variables in the principal plan

Principal Components Analysis attempts to describe the relationship between input variables. This is done by building a new basis characterised by non correlated axis. Each axis is given a level of importance. The behaviour of input variables regarding these axis is then studied to describe multiple dependencies between input variables.
Considering 5 axis in the PCA, input variables are represented at a level of 90% [3]. First axis explains 40% of the whole variability. It illustrates a strong positive correlation between variety and temperature. The first axis also shows that temperature and variety vary in the opposite to rainfall. The second axis shows a positive dependency between radiation and evapotranspiration and a negative one between these and rainfall.

As shown above, evapotranspiration and radiation are strongly correlated. Because both are important in crop physiology, both will be kept in the analysis. One will be fitted to the other and then replaced by the residuals of the regression. In the successive statistical analysis, radiation will bring only information about itself and not about evapotranspiration.

3 SENSITIVITY ANALYSIS METHOD : DETERMINATION OF INFLUENCE

Sensitivity analysis involves determining the contribution of individual input variables on output predictions.
Evaluated outputs will be the values of the following indicators when crop maturity is reached :

- Total biomass of the plant (Kg/ha) obtained either in water limited condition (**BW**) or in optimal condition for water (ie. irrigated) (**BP**).
- Storage organ (Kg/ha) available either in water limited condition (**SW**) or in optimal condition for water (ie. irrigated) (**SP**).

Only real observed input data and their corresponding output predictions are used in this analysis to determine the level of influence through multiple evaluations. No simulated sets of input or output data have been used. Sensitivity indicators refer to the technique of analysis of variance. When considering all variables, the sensitivity model is described by Eq.1.

Eq.1 $Y = \beta_0 + \beta_1 temp + \beta_2 rad. + \beta_3 ETp + \beta_4 rain + \beta_5 variety + \beta_6 SPG + \beta_7 RD$

where β_n are the standardised estimated coefficients [4] (i.e coefficients of influence). The higher their absolute value, the more influence the corresponding input variable has on output predictions. A negative value indicates that input and output vary in opposite direction.
The stepwise method is used to select explanatory variables. Levels of priority are assigned to each candidate, then variables are stepwisely tested for significance to determine their contribution in the final sensitivity model. Because the sensitivity model requires quantitative variables, categorical ones such as (soil characteritics and variety) are recoded and transformed into quantitative ones by considering the mean of the output for each level instead of the level itself. Candidate variables are then introduced separately and tested for for their influence.

Clustering
Original data were too scattered and not discriminated enough by meteorological variables, they have been clustered to increase the quality of the linear regression model.

K-means algorithm is used to create homogeneous groups from the 4 meteorological variables array. From randomly initial kernels I_k, k=1,.. n_{class}, classification will consist in minimising distance between the units values and the centre of the class. The procedure is repeated until two successive steps leave the clusters configuration unchanged. In the end, 51 classes were created. The input array for the sensitivity analysis is then formed with the combination of the 51 meteorological classes and the possible factors for soil and variety.

Input Array = 51 Meteorological clusters x Soil factors x Variety

The influence of these inputs values are tested in the sensitivity model (Eq. 1), the output values being the average yield for each input cell array

4 RESULTS AND INTERPRETATION

Table 1: Global sensitivity on CGMS

	High Influence	Medium Influence	R2 %
SW	Variety, Soil Depth, Evapotranspiration	Rainfall	71.95
SP	Variety	Radiation	70.97
BW	Variety, Soil Depth	Soil Group, Evapotranspiration, Temperature, Rainfall	59.42
BP	Evapotranspiration, Variety, Radiation	Temperature, Soil Depth	35.14

Variables are underlined in the table when input and output behaviour are opposite (negative value for β in Eq1).

Storage organ in water limited condition (SW) are well-represented by explanatory variables (72%). Variety and soil depth having the highest sensitivity indicator. Within meteorological variables, evapotranspiration has also a strong negative sensitivity indicator (high evapotranspiration will decrease storage organ weight). Rainfall has only a medium influence.

Under optimal water regime, 70% of the storage organ weight (SP) is explained mainly by 2 variables (variety and radiation). Variety being the only parameter to have a strong influence.

Biomass in water limited condition (BW) is sensitive to all variables related to variety and soil. Meteorological variables having only a medium or low influence.

Biomass in optimal water condition (BP) is the output variable least influenced by input data (only 35%). Due to the low regression coefficient, results should be interpreted with care, especially the influence of evapotranspiration not relevant in optimal water regime.

5 DISCUSSION

Grain and biomass production are both strongly dependant on CGMS variety tuning factor. This first result illustrates the importance of validating the crop cycle length and the crop calendar used by the model. It also highlights the importance of precise determination of sowing date to start the crop growth model.

In water limited condition, input variables related directly to soil water balance calculation have the highest influence (soil depth, rainfall). Future improvement of the CGMS soil module should consider the preponderance of soil depth compared to soil type while both are used in the calculation of the available water in the soil

Amongst meteorological variables, evapotranspiration and radiation are the most influential ones.

6 CONCLUSION

The sensitivity analysis carried out on the Crop Growth Monitoring System has permitted to identify the input features (i.e. variety and soil depth factor) having the largest influence for the yield of wheat crop. This analysis, taking into account the spatial variation of input parameters, is the first step towards the full understanding of the model's mechanism.

Further analysis is now required to consider temporal effects of input parameters on crop yield results. It could be done by using logistic functions. Concerning the relative poor results on biomass, an attempt should be made by simulating input data into reasonable range of values and by using Monte Carlo method to evaluate the results.

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ON THE SENSITIVITY OF OPTIMAL MACROECONOMIC POLICIES WITH RESPECT TO STOCHASTIC MODEL PARAMETERS: A CASE STUDY FOR AUSTRIA

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1 INTRODUCTION

For a long time, there has been an intensive debate in economics whether fiscal and monetary policies should l used to influence macroeconomic variables such as employment, output, the price level, and the extern balance. In particular, monetarists have argued against the discretionary use of budgetary and monetary polici for stabilization purposes because of long lags and of the uncertainty about the effects of these policies on t economy. Even if one is ready to accept a theoretical position implying potential effectiveness of stabilizati policies, the argument of limited knowledge about policy effects has to be taken seriously when designing actu policy measures. Some theoretical work has been done on the influence of uncertainty upon the design macroeconomic policies (e.g., [1], [2]). It shows that policy uncertainty can be captured in macroeconom models by assuming the model parameters to follow some probability distribution and deriving optimal values time paths of policy variables in such a stochastic setting. The analytical results obtained in this literature a necessarily based on rather restrictive assumptions and do not yield conclusions which could be readily appli to actual policy problems. Therefore, numerical results are desirable for such a purpose, which should be bas on econometric models estimated from actual data for the economy to which fiscal and monetary policies are be applied. In this paper, we analyze some of these issues within a problem of quantitative economic polic using an optimum control approach.

2 DESIGN OF THE EXPERIMENTS

In order to examine the sensitivity of optimal policies to stochastic parameters, we first determine numerica optimal fiscal and monetary policies for Austria for the nineties by minimizing an intertemporal objecti function subject to the constraints given by an econometric model. The model, called FINPOL2, is a mediu size macroeconometric model for Austria. It relates policy and exogenous variables to objective variables Austrian economic policies, such as the rate of unemployment, the rate of inflation, the growth rate of real GL the current account and the budget deficit. The model FINPOL2 is based on traditional Keynesi macroeconomic theory in the sense of conventional IS-LM/aggregate demand-aggregate supply mode Stochastic behavioral equations for the demand side include a consumption function, an investment function, import function and an interest-rate equation as a reduced-form money market model. Prices are larg determined by aggregate demand variables. Disequilibrium in the labor market, as measured by the excess unemployed persons over vacancies, is modelled to depend on the real GDP growth rate and the rate inflation, embodying both an Okun's law-type relation and a rudimentary Phillips curve. The model, which dynamic and nonlinear, was estimated by 3SLS using annual data over the period 1965 to 1992. For details the model equations, see [3].

Moreover, we postulate an objective function for Austrian policy-makers over the years 1993 to 20 which penalizes deviations of objective variables from their desired values. The objective function is quadra in the deviations of the state and control variables from their respective desired values. Among the variab whose deviations from desired values are to be penalized, we assume that there are five "main" object variables which are of direct political relevance in assessing the performance of the Austrian economy. Th are the rate of inflation ($PV\%_t$), the labor market excess supply variable (UN_t) as a measure for involunt unemployment, the rate of growth of real GDP ($YR\%_t$), the current account (LBR_t), and the federal net bud

deficit as percentage of GDP ($DEF\%_t$). In all experiments, 2% p.a. is considered as the desired rate of inflation ($PV\%_t$), 3.5% p.a. as the desired real growth rate ($YR\%_t$), and the desired levels for labor market excess supply (UN_t) and the current account (LBR_t) are set equal to zero. For the deficit variable, we assume that the aim is to consolidate the federal budget deficit gradually such that the desired value of $DEF\%_t$ is reduced by 0.3 percentage points each year, from the historical value of 3.27% in 1992 down to 0.87% in 2000. Moreover, several other variables are used as "minor" objective variables, which mainly serves as a substitute for imposing inequality constraints on state and control variables to prevent erratic fluctuations of these variables. In the weight matrix of the objective function, all off-diagonal elements are set equal to zero, and the main diagonal elements are given weights of 10 for the "main" objective variables and of 1 for the "minor" objective variables. The weight matrix is assumed to be constant over time.

The exogenous variables of the model are forecast over the planning horizon using time series methods. Here we use extrapolations of these variables for the years 1993 to 2000 calculated from linear stochastic time series models of the ARMA (mixed autoregressive-moving average process) type. After several trials and applying the usual diagnostic checking procedure for the time series under consideration, we decided to model the control (instrument) variables federal budget expenditures (NEX_t) by an ARMA (2,1) process, federal budget revenues (BIN_t) by an ARMA (2,2) process, and money supply ($M1_t$) by an ARMA (2,1) process, and the non-controlled exogenous variables import price level (PM_t) by an ARMA (1,1) process, real exports of goods and services (XR_t) by an ARMA (2,3) process, and the inventory change variable IIR_t by an AR (1) process.

3 RESULTS OF OPTIMAL POLICY EXPERIMENTS

As a first step, the model was simulated over the years 1993 to 2000 using the extrapolations of all (controlled and non-controlled) exogenous variables from the time series models as input. Next, we calculated optimal stabilization policies over this time horizon using the stochastic control algorithm OPTCON. Here again the projections of the non-controlled exogenous variables from the time series models are used as inputs, being assumed to be known for certain, but the values of the policy instruments are determined endogenously as (approximately) optimal under the assumed objective function. For a deterministic optimization run, we assumed all parameters of the model to be known for certain. This amounts to a neglect of uncertainty of all policy effects. For a fully stochastic optimization run, on the other hand, only deterministic paths for the non-controlled exogenous variables were assumed, but the estimated covariance matrices of the parameters and of the additive disturbances of the model, which are obtained from the 3SLS estimation, are taken into account when calculating optimal policies.

As shown in [3], the projection scenario results in rather optimistic forecasts. In spite of the already optimistic picture of the future development of the Austrian economy provided by the projected forecast, there is still some scope for optimal stabilization policy, as can be seen from the two optimization experiments. In particular, optimal fiscal and monetary policies are more countercyclical than projected ones and imply smoother time paths of the endogenous variables of the model.

There is not much difference between the deterministic (Table 1) and the fully stochastic (Table 2) optimization run. Optimal values of budgetary policy variables are close in these two experiments, with more expansionary policies (higher NEX_t, lower BIN_t) in 1993, 1996, and 1998, and more restrictive policies (lower NEX_t, higher BIN_t) in 1994, 1995, 1997, and 2000 in the fully stochastic optimum; in 1999, both NEX_t and BIN_t are higher in the stochastic optimization run. Optimal monetary policy is always slightly more restrictive ($M1_t$ is lower) in the stochastic solution. The optimal value of the objective function is 125,810.2 in the deterministic experiment and 151,027.9 in the fully stochastic one; hence the costs of uncertainty are about 20% of the deterministic minimum costs, which seems rather small.

The similarity between the optimal deterministic and stochastic paths of budgetary and monetary policies seems to imply that optimal policies are reliable even when neglecting parameter uncertainty. This is somewhat astonishing, because previous theoretical and numerical studies using simple macroeconomic models have shown that uncertainty generally matters in the design of optimal stabilization policies. Therefore we would like to know whether our result holds true also when only some parameters of the model are treated as stochastic, with the other ones remaining deterministic. To do so, we introduced different assumptions about parameter uncertainties into our model FINPOL2 in order to assess the influence of various kinds of uncertainty on the design of future optimal budgetary and monetary policies. In particular, we investigated the effects of making several key parameters determining fiscal and monetary policy multipliers uncertain.

Table 1: Optimal Values of Instruments and "Main" Objectives, Deterministic Optimum

year	NEX_t	BIN_t	$M1_t$	$PV\%_t$	UN_t	$YR\%_t$	LBR_t	$DEF\%_t$
1993	734.641	581.421	326.892	2.063	4.807	1.996	-22.144	7.196
1994	769.752	639.456	340.949	2.597	4.112	4.632	-7.253	5.671
1995	789.774	698.940	355.651	2.753	3.454	4.943	9.858	3.644
1996	833.577	746.124	373.033	2.658	3.428	3.365	12.669	3.282
1997	870.066	806.048	390.509	2.712	3.278	3.769	22.733	2.238
1998	907.822	870.236	409.455	2.681	3.279	3.390	32.310	1.229
1999	937.960	934.985	430.907	2.692	3.245	3.502	44.772	0.091
2000	959.630	974.370	457.717	2.838	2.920	4.423	55.274	-0.416

Table 2: Optimal Values of Instruments and "Main" Objectives, Fully Stochastic Optimum

year	NEX_t	BIN_t	$M1_t$	$PV\%_t$	UN_t	$YR\%_t$	LBR_t	$DEF\%_t$
1993	737.491	578.554	326.768	2.098	4.721	2.267	-22.936	7.442
1994	769.138	640.722	339.900	2.585	4.120	4.389	-7.919	5.585
1995	787.776	700.849	354.465	2.724	3.529	4.726	9.944	3.493
1996	834.411	745.503	372.107	2.660	3.450	3.485	12.915	3.339
1997	869.633	806.577	389.416	2.705	3.302	3.750	23.166	2.207
1998	908.032	869.839	408.408	2.684	3.279	3.451	32.677	1.249
1999	938.576	936.298	429.693	2.690	3.248	3.493	45.132	0.070
2000	957.613	983.276	456.251	2.784	3.032	4.085	56.884	-0.728

As our model FINPOL2 was estimated by 3SLS, we have an estimate of the entire parameter covariance matrix. To concentrate upon the effects of uncertainty of some key parameters, we neglect the variance and covariance estimates of the other parameters. However, it turns out that taking into account or not covariances between different parameters may be crucial for optimal policies. Therefore, in a series of experiments, we calculated three versions of optimal macroeconomic policies. For Version A, only the variances of the parameters being regarded as stochastic were taken into account and all covariances were neglected. In this case, the parameter covariance matrix is diagonal, with non-zero elements in the main diagonal only for the stochastic parameters. Version B takes into account also the covariances between the parameters with non-zero variances. For Version C, in addition all covariances between the stochastic parameters and all other parameters (which still have zero variances) are given non-zero values. In this way, we want to study effects of correlations between parameter estimates on the design of optimal policies. Estimates for parameter variances and covariances were always taken from the estimated parameter covariance matrix obtained from the 3SLS estimation. Detailed results are available upon request; here we show only one example and the general conclusion.

In general, it turns out that optimal monetary and especially budgetary policies and their performance depend upon the amount of correlations between the stochastic parameters of the model. This can be seen from the results of an experiment where we assume all estimated parameters of the model to be stochastic but neglect their covariances, i.e., we only take into account the estimated own variances of the 37 parameters. This can be regarded as Version A of a fully stochastic optimization experiment; Versions B and C are identical to the fully stochastic optimum (Table 2). Results are shown in Table 3. Here, optimal budgetary policies are dramatically different from both the deterministic ones and the fully stochastic ones with parameter covariances taken into account. High federal budget tax revenues and low federal budget expenditures combine to create a budget surplus for all but one year. These restrictive fiscal policies are mitigated by slightly more expansionary monetary policies (except for 1993), but the values of $M1_t$ are closer to previous ones than those of fiscal instruments. A severe recession is created in 1993, with real GDP falling by more than 12% and labor market excess supply jumping up to more than 9%. Intertemporal trade-offs are exploited to some extent, because UN_t comes down to 1.6% until 2000, inflation remains low, and the current account has a big surplus in every year, but the overall performance is severely deteriorated, with an optimum value of the objective function of 10,629,681.6. We have to conclude that neglecting parameter covariances in stochastic optimization problems results in optimal policies which are heavily biased as compared to the "true" (approximate) fully stochastic optimum with parameter covariances taken into account.

Table 3: Optimal Values of Instruments and "Main" Objectives, Stochastic Optimum, Version A

year	NEX_t	BIN_t	MI_t	$PV\%_t$	UN_t	$YR\%_t$	LBR_t	$DEF\%_t$
1993	706.010	849.255	323.353	0.205	9.379	-12.316	19.780	-7.971
1994	835.922	807.122	346.738	1.567	7.912	4.355	67.193	1.514
1995	868.095	874.656	360.436	1.919	6.233	5.962	107.170	-0.319
1996	907.482	937.512	375.562	1.973	5.452	4.172	125.792	-1.371
1997	931.912	1008.076	391.679	2.111	4.821	4.175	147.858	-3.255
1998	955.037	1065.136	411.494	2.227	4.333	4.106	165.519	-4.400
1999	967.579	1093.403	435.938	2.536	3.460	5.596	178.757	-4.618
2000	979.881	1056.394	464.730	3.255	1.564	9.290	175.313	-2.473

4 CONCLUSIONS

The results of our experiments show that optimal macroeconomic policies for the particular model employed are very sensitive with respect to stochastics affecting policy multipliers and especially to correlations of these parameters with other ones. On the other hand, if the full covariance matrix of the parameters is taken into account, optimal policies are similar to those obtained in the deterministic case. We interpret this result as showing the reliability of optimal policy recommendations when the full covariance matrix is either taken into account or totally neglected, i.e., deterministic optimal policies can be relied upon even in a world of uncertainty. On the other hand, neglecting correlations between model parameters leads to policy recommendations which ought not to be presented to policy-makers as they are seriously flawed. This result is important for practical policy advisers, because often econometric models are estimated by OLS, hence no estimate for the entire parameter covariance matrix is available. In this case, results based on deterministic optimization are to be preferred to those based on rudimentary stochastics.

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SENSITIVITY ANALYSIS OF RELIABILITY INDICES ON STATION INITIATED FAILURES IN COMPOSITE POWER SYSTEM RELIABILITY EVALUATION

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1 INTRODUCTION

The reliability evaluation of a composite power system usually considers the outage impact of generating units, transformers, overhead transmission lines and cables only. The power system buses are assumed to be perfectly reliable and fully capable, which is not the case in the real power system. A bus (node) in power network is actually a terminal in the power substation having many components such as circuit breakers, bus sections, disclosures, station power transformers and protective relays. The outage impacts of these components on the power system can have a significant effect, and therefore, should not be ignored. The failures of substations devices are a major cause of multiple components outages [1]. This paper will present sensitivity analysis of reliability indices of power substations on station initiated outages and illustrate the effects of terminal station outages on the power system performance. The principle of the substation reliability computation is based on Markov model of components and on enumeration of the states of all major components in a switching substation, i.e. bus sections, circuit breakers, station transformers, series capacitor, reactors, generating units or cables. Bus sections and station transformers are assumed to be either completely operable and available or completely down and unavailable.

2 MATHEMATICAL MODEL

The reliability indices of substation are computed using Markov model, which indicates the transition rates between the various component's states [2]. Bus section and transformer are modelled with two states, the up state and the down state, so that only two parameters are required to describe the model completely. These are the failure rate (λ) and the repair rate (μ), from which we can compute the probability of residing in either up or down state. Circuit breakers have many models of failure, three of which are used in this evaluation. The first failure mode is a breaker failure due to a fault from line to ground, the second is a so-called "stuck breaker" mode, and the third is a faulted breaker.

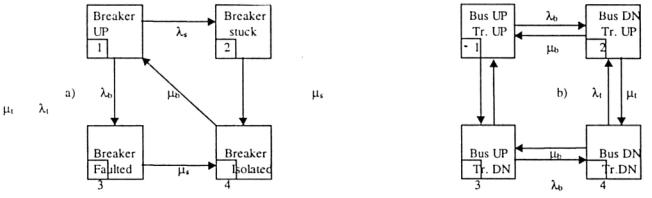

Figure 1: Markov models of circuit breaker (a) and of overlapping failure of bus section and transformers (b)

The list of outage events considered in the study of substation related failures includes:

1. Stuck breaker outage: a fault on the line/generating unit followed by the stuck breaker condition.
2. Bus section outage: a fault on a bus section.
3. Station transformer outage: a fault on station transformer.
4. Maintenance overlapping forced outage: for bus section or transformer
5. Overlapping forced outage: for bus section or transformer

There are some assumptions used in Markov model. Probability of overlapping outage for three or more components is assumed to be zero. A component is not taken out of service, for preventive maintenance, if it results in the outage of a current carrying component. Failure bunching effects due to adverse weather are not considered. Reliability indices calculated by this analysis are:

1. Bulk Power Supply Disturbance (BPSD):

$$BPSD_{Probability} = \sum_j P_j \quad (1)$$

$$BPSD_{Frequency} = \sum_j f_j \text{ [occ/yr]} \quad (2)$$

$$BPSD_{Duration} = \sum_j D_j \cdot f_j \text{ [hrs/yr]} \quad (3)$$

2. Expected Energy Not Supplied (EENS):

$$EENS = \sum_k \sum_j P_j \cdot L_{kj} \text{ [MW/occ]} \quad (4)$$

3. Severity Index (System Minutes, SM):

$$SM = \frac{60 \cdot \sum_k \sum_j L_{kj} \cdot D_{kj} \cdot f_j}{L_S} \text{ [Sys-Min]} \quad (5)$$

where: P_j = state probability of outage event j
f_j = frequency of occurrence of outage event j
D_j = duration in hours of the load curtailment arising due to contingency j
L_{kj} = load curtailed at bus k due to contingency j
L_S = total system load in MW.

3 SAMPLE CASE

This paper describes a sensitivity analysis of the reliability evaluation of a transmission switching station in a sample case of power system. Requirements for the calculation are station topology data, protection data, reliability data (i.e. failure and repair rates, repair time, etc.) and of course power system data. All computations are performed on the RTS one-line diagram of a 24-bus test power system described in [3]. 3405 MW capacity is installed with a system peak load of 2850 MW. The RTS system was developed by IEEE task force as a reference network.

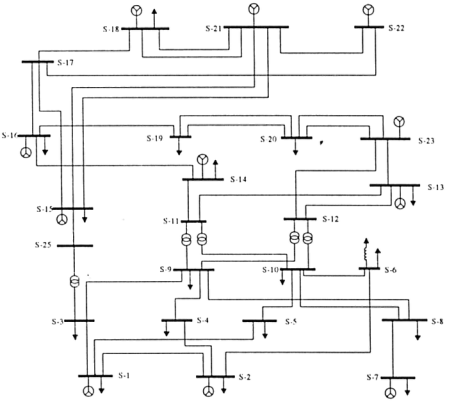

Figure 2: A sample case of IEEE-RTS power system

In order to incorporate switching and substations in a composite generation and transmission analysis, each station must be analysed separately with the STAREL program [4].

The reliability analysis of station initiated outage events includes a number of probabilistic indices, such as:

1. The probability, frequency and duration for each station originated outage event.
2. The probability, frequency and duration of electric power system components terminated on a station which are outaged due to the failures of station components.
3. The minimum availability index for each station configuration.
4. The expected power and energy curtailed (i.e. not served to the load which is connected on the station).

The main goal of the paper is to investigate the influence of a breaker repair rate and of breaker isolation rate on reliability indices. These two rates depend on the station topology and on the level of automatization in the station and vary from case to case. For all these calculation authors have used the "STAREL" computer program [4]. Outage events are simulated on stations located at bus S-3 whose configuration is not certain and on a ring bus S-13 whose configuration is shown in figure 3, from [5].

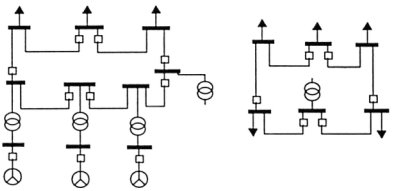

Figure 3: Station configurations: ring bus 13 and 3

4 RESULTS OF THE ANALYSIS

Reliability evaluation of the RTS system with and without the station originated outages is performed on 2nd contingency level of both generators and branches. The influence of station originated events on reliability indices was computed only for terminal station on bus 3 and 13. Comparison is shown in table 1.

Table 1: Influence of station outages on reliability indices

Reliability indices	Without station outages evaluation	With station Outages evaluation	Increasing precentage
BPSD Probability	0.010009	0.012098	20,87%
BPSD Frequency (occ/yr)	4.653363	4.690946	0,81%
BPSD Duration (hrs/yr)	87.680145	105.978210	20,87%
Severity Index (Sys-Min)	212.443420	317.528320	49,46%
EENS (MWh/occ)	24.741835	195.948059	691,97%

In order to determine the sensitivity of reliability indices on repair and planned maintenance time, authors performed analysis with different repair and maintenance time of the following station components: breakers, station transformers and bus sections. Basic values for those times are accepted from [4]. To decrease a computation time, all of these sensitivity analysis results are computed on 1st contingency level of generators and on 2nd contingency level of branches. Reliability indices of the RTS system are very sensitive on the influence of the station originated events. When the time to repair of a station component is 20% less or 20% above the basic value BPSD Probability index decrease or increase respectively. The effect of maintenance time changes is negligible.

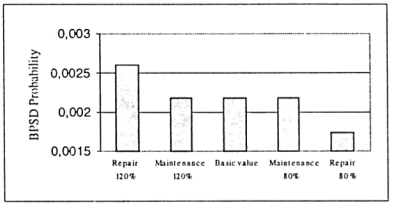

Figure 4: Sensitivity of BPSD Probability on changes of repair and maintenance time

In the case of BPSD Frequency index, when the time to repair is 20% less, working time of the components is longer, hence they are potentially more exposed to all failures, and this is a reason for frequency increasing and vice versa. But, when the maintenance time decreases for 20%, BPSD frequency decreases. This results from the fact that the total frequency of coincidence between failure and maintenance depends on a maintenance time.

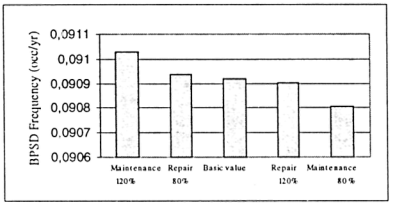

Figure5: Sensitivity of BPSD Frequency on changes of repair and maintenance times

Figure 6 represents the sensitivity of EENS index, which is respective to the changes of BPSD Probability, according to the equation (4).

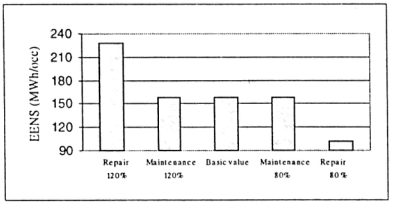

Figure 6: Sensitivity of the EENS on the changes of repair and maintenance times

Comparison of Figure 4. and Figure 6. indicates changes of reliability indices BPSD Probability and EENS in the same manner. That is the case with BPSD Duration and Severity index as well as most of the reliability indices which are calculated during this analysis.

5 CONCLUSION

In this paper sensitivity analysis of reliability indices on station initiated failures in a composite power system reliability evaluation is presented. Two powerful program packages "COMREL" and "STAREL" are used for computation of several reliability indices. The results of the analysis indicate great influence of station originated outages on all reliability indices. Station originated events must be included when reliability assessment of power system is performed. The influence of time to repair and maintenance time on reliability indices is investigated.

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WHEN GOOD MODELS ARE FALSE: SOBERING LESSONS FROM THE HISTORY OF SCIENCE

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1 INTRODUCTION

Sensitivity analysis is one of the most valuable uses of numerical simulation models. By permitting modelers to ask "what if" questions, sensitivity analysis can illuminate which aspects of a system are most in need of further study. [1] A question that arises in modeling, however-indeed in all science-is the accuracy of the underlying conceptualization. Given a particular conceptualization of a system, sensitivity analysis can help us improve our understanding of that system, so conceptualized. But how do we know if the conceptualization is correct, or even approximately so? The normal assumption of most scientists is that correct ideas make correct predictions. If a model generates output in conformity with observable variables, then it seems reasonable to assume that the model is more or less on track.

Are we right in this assumption? Scientific experience suggests in most cases yes. Many models work well, and as we find out more about the world we need to refine them, but we don't often have to revamp them totally. The history of science, however, tells a less reassuring story. Scientists in the past have sometimes had faith in conceptual models that accurately predicted empirical outcomes, yet subsequently were shown to fail in correspondence with the physical world. In this paper, I discuss
one example: the problem of isostatic compensation and its relation to the question of continental drift.

2 ISOSTASY AND CONTINENTAL DRIFT

Most scientists are familiar with the work of Alfred Wegener, the German meteorologist and geophysicist (1880-1930) who in the early twentieth century proposed the theory of continental drift. By his own account, Wegener wanted to explain the well-known 'jigsaw-puzzle fit' of the continents; he suggested that they were once contiguous and had broken apart in relatively recent geological times. Geological evidence provided corroboratation: the fossil assemblages and stratigraphic successions of South America and Africa were strikingly similar throughout nearly 200 million years of Mesozoic history. In the nineteenth century, these parallels had been explained by the theory of Gondwana: a ancient supercontinent presumed to have broken apart in response to terrestrial thermal contraction. The missing pieces of Gondwana were thought to have sunk beneath the oceanic depths.

Wegener was impressed with the apparent unanimity of paleontologists in their demands for prior land connections. But there was a problem: Geophysics would not permit the sinking of continents. In 1909-1912 American geophysicists John Hayford and William Bowie demonstrated on the basis of geodetic and gravity measurements that the earth's crust floats in hydrostatic equilibrium upon a denser substrate-an idea known as isostasy Isostasy directly contradicted the theory of Gondwana: if continents are less dense than their substrate, they cannot sink into it. Wegener thus proposed continental drift as a reconciliation between the facts of historical geology and the constraints of isostasy, and one might therefore suppose that geodesists would have been among his stronges supporters. But geodesists, led by Bowie, strongly opposed the theory. In a letter written in the autumn of 1928 Bowie argued that continental drift was impossible, even given the recent work of Arthur Holmes in suggesting the role of sub-crustal convection currents in driving continental motions.

> "I really cannot figure out how the continents can drift about in an aimless sort of way [Bowie wrote]. Holmes brings out a new thought which is even more impossible than Wegener's hypothesis. That is that the submerged ridge through the Atlantic Ocean is the place at which North and South America separated from Europe and Africa, the latter two continents drifting eastward and the Americas drifting westward....I believe that we need to apply elementary physics and mechanics to the continental drift problem in order to show how impossible that drifting would be." [2]

Holmes's 'new thought' was mantle convection, which is generally accepted today as the driving force of plate tectonics. Why did Bowie think that convection causing horizontal movements was impossible? The answer is revealed in another letter: "If we have the Airy isostasy," Bowie acknowledged, "then there must have been horizontal movements forming roots to the topographic features."[3] Bowie was referring here to the fact that there were two different models of isostatic compensation, both of which were consistent with geodetic evidence. In 1855 British Astronomer Royal George Biddell Airy suggested that isostasy could be achieved if the continents had roots, like icebergs at sea (Fig. 1). In 1871 John Henry Pratt argued that isostasy could be equally well achieved by subterranean density differences that compensated for above-ground topography (Fig. 2). Conceptually, the two models were radically different, but mathematically they were equivalent.

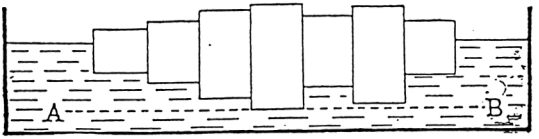

FIG. —An illustration of isostasy after the Airy, or Roots of Mountains, principle. In this case the blocks are of the same material, copper, have the same cross section but different lengths; each has a different mass, hence their surfaces extend to different depths in the mercury and extend upward to different heights. This should be contrasted with Fig. 4, which illustrates the Pratt idea of isostasy. From article by C. R. Longwell, *Geographical Review*, January, 1925.

Figure 1 The Airy model of isostasy

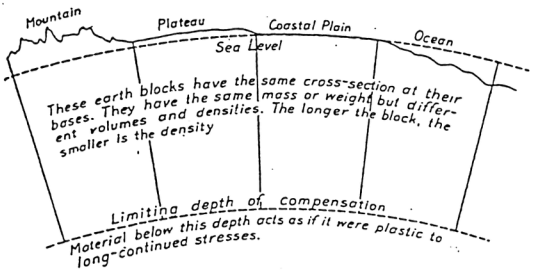

FIG. —If the earth's crust should be cut into blocks of equal horizontal cross section by vertical planes, each block would have very nearly the same mass as each of the other blocks. The blocks would exert the same pressure on the subcrustal material. It is not definitely known what is the cross section of the block which may be in isostatic equilibrium independently of the surrounding blocks but it is probably of the order of magnitude of 50 or 100 miles square.

Figure 2 The Pratt model of isostasy

Crustal roots implied lateral compression to create and sustain them. Continental drift and the Airy model thus seemed to go hand-in-glove. But Bowie subscribed to the Pratt model; he and Hayford had used it as the basis of their demonstration of isostasy. Why did they chose Pratt over Airy? The answer is not a mystery. In The Figure of the Earth, Hayford's seminal work, he wrote: "The assumption [of Pratt isostasy] was adopted as a working hypothesis, because it happens to be that one of the reasonable assumptions which lends itself most readily to computation." (4) Hayford did what all scientists are taught to do: He applied Ockham's razor. Given two possible interpretations, he used the simplest one-simplicity in this case being defined as ease of calculation. But this methodological choice had theoretical implications. It was incompatible with continental drift. Because the Pratt model worked, Bowie assumed that it was correct, and therefore that continental drift was not.

3 CONCLUSION

In retrospect we can see the obvious error of Bowie's logic, but why else do scientists accept the veracity of their models? Scientists accept models and theories because they work: because they explain things that weren't explained before, because they make correct predictions, or because when one accepts them as true, one can solve problems that couldn't be solved before. This is what Bowie did. But the difficulty is obvious: It is the logical fallacy of affirming the consequent. False theories sometimes work. The Ptolemaic system of astronomy enabled scientists to predict the motions of the planets, and the Pratt model enabled John Hayford and William Bowie to calculate the isostatic adjustment and gravitational anomalies of the United States.

My purpose in presenting this historical episode here is not to be discouraging, but simply to pose the following question: Could sensitivity analysis have uncovered this problem? And if not, what tools do modelers have to determine whether or not their conceptual models are right?

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COMPARISON OF GLOBAL SENSITIVITY TECHNIQUES FOR THE ANALYSIS OF A SHALLOW-WATER 3D EUTROPHICATION MODEL

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1 INTRODUCTION

The concern about the pollution of coastal areas has prompted a large number of field and modelling studies on the dynamic of these environments, which are also considered as important economical resources. Among them, lagoons and shallow-water estuaries occupy an important place because they can be exploited for recreational purposes and also for their great potential primary productivity, which could be «channelled» through the trophic chain up to levels of economical interests, as mussels and fish.

The dynamic of these transition systems is very rich as they receive inputs of mechanical energy (e.g. tide and wind), solar free energy and nutrients (mainly Nitrogen and Phosphorous). These inputs stimulate the primary production both in the water column and at the bottom of the lagoons: opposite to pelagic systems, the bottom is not only a sink but acts as an important source of nutrients because of the shallowness and of the vertical turbulence caused by wind and tidal agitation. As a result, these ecosystems show strong spatial gradients, i.e. of salinity from the river mouth to the sea, of Dissolved Oxygen (DO) from the surface to the bottom, which makes it hard to describe by means of lumped parameter models, i.e. ordinary differential equations.

Despite of the shallowness of these environments, the presence of strong vertical gradients is evident in some instances. For example, the high level of turbidity cause a big reduction of the availability of solar energy, which in turn can lower the photosynthetic activity along the vertical, while bacterial decomposition of organic detritus causes the depletion of the concentration of DO at the sediment-water interface. For this purpose, the seasonal evolution of the system has been followed by means of a simple 3-dimensional model, which mimics the main features of a shallow estuarine environment. With this model, it is possible to catch the main dynamic features at reasonable computational costs, which enable us to use global approaches to sensitivity analysis.

2 THE MODEL

This section outlines the model which describes the dynamic of the phytoplanktonic and macro-algal communities in a shallow water estuary, has been developed as part of a long-term study to investigate the problem of eutrophication in the lagoon of Venice ([1],[2],[3]). During the eighties, the lagoon was invaded by macroalgae, *Ulva rigida*, which greatly affected the oxygen balance in the shallowest areas. After reaching their maximum at the end of the eighties, the population of these macro-algae started a fast decline, particularly evident in the central part of the lagoon. This was triggered by a change of the climatic conditions, especially during the spring, [4].

The 3-D model mimics the essential spatial features of the whole central part of the lagoon, [5]. In fact, this part of the lagoon can be regarded as a shallow basin surrounded by two main canals, which are connected at the mouths of Lido and Malamocco. The open boundary conditions are chosen according to interpolation of experimental data collected at the mouth of Lido and of Malamocco. The model follows the dynamic of twelve state variables: they are densities of *Ulva rigida*; phytoplankton and zooplankton; concentrations of internal Nitrogen in *Ulva*; Nitrogen (N) and Phosphorous (P) in the water column, in the organic detritus and in the

upper sediment; DO and water temperature. The non-linear system, which describes their dynamic, has been discussed in details (see [5]). Transport processes are simulated by turbulent diffusion with a constant diffusivity along the vertical and horizontal diffusivities which vary according to the depth and the geometry of the bathymetry, [6].

3 SENSITIVITY ANALYSIS (SA)

The model outlined in Section 2 can be thought of as the superposition of two trophic models: the first describes the dynamic of the phytoplanktonic community and the second the one of benthic macro-algae. Both models have been investigated separately by means of a local sensitivity analysis, [7], which gave an initial idea of the most important processes. The full model will be investigated here by means of global sensitivity techniques to understand how the total yearly biomass production and the lowest oxygen level are affected by the input parameters. Previous studies have suggested, at qualitative level, that groups of parameters may interact strongly with each other and hence affect the dynamic of the two communities. Such effects cannot be detected by local sensitivity analysis but can be highlighted by performing global sensitivity analysis.

In global sensitivity analysis, the input parameters are allowed to vary over a finite (or even infinite) range. In this paper, the usual measure, (Pearson Correlation Coefficient, Spearman Correlation Coefficient, Partial Correlation Coefficient, Partial Rank Correlation Coefficient, Standardised Regression Coefficient, Standardised Regression Coefficient etc.), are computed and results are compared with those obtained by a variance based method. In particular, Sobol' methods, [8], will be applied to the problem described above. This method, as well as the other based on variance decomposition, not only can measure the «main effect» (or the so-called first order term) contribution of each parameter to the output variance, they can also compute the so-called «Total Sensitivity Indices» (*TSI*). The Total Sensitivity Index of parameter i, denoted by $ST(i)$, is defined as the sum of all the sensitivity indices (including all the interaction effects) involving parameter i, [9]. For example, suppose that there are only three input parameters (A, B and C) in our model. Figure 1 illustrates that the total effect of parameter A, for instance, in the output is given by

$$TS(A) = S(A) + S(A,B) + S(A,C) + S(A,B,C),$$

where $S(A)$ denotes the so-called first order sensitivity index for parameter A, $S(A,j)$ denotes the second order sensitivity index for the parameters A and j (for j not equal A), i.e. the interactions between parameters A and j (for j not equal A), and so on.

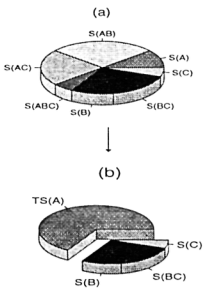

Figure 1: Graphical Representation of (a) Sensitivity Indices for the Three Parameters Case and (b) Total Sensitivity Indices of Parameter A

For management purposes, one is particularly interested in finding out the combined effects of parameters related to uncontrollable inputs (i.e. solar radiation, and turbulence), or to controllable ones (i.e. nutrient loads). Preliminary results suggest that, on a mid-term basis, meteoclimatic parameters may be more important than controllable ones and can trigger the appearance of new species or the decline of existing ones in the ecosystem, as has happened for the macroalgal species, *Ulva rigida*.

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FEEDFORWARD NEURAL NETWORKS SENSITIVITY TO INPUT DATA REPRESENTATION

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1 INTRODUCTION

Since McCulloch and Pitts (1) proposed the "switching element" as a first computational model of a brain cell, the artificial neural networks (ANN) began to be widely used. After the development of error back-propagation learning algorithm, the feed forward layered ANN is the most widely used architecture. Attractiveness of ANN's stems from the fact, that to solve a given problem, one does not necessarily need to wholly understand the underlying problem, but only how to learn.

Among the tasks ANN's perform are (2): approximation of linear mappings, time–series prediction, process control, association of patterns, spatial filtering of signals in a noisy environment, and pattern classification.

The patterns that are to be classified, since single ANN cells process only numerical signals, have to be given as number vectors. This is all too well in problems with physical background. But ANN's can also be used to solve tasks which are purely symbolic in nature. There, one has to find a mapping from the set of symbols used to a space of real numbers of a given dimension.

$$mapping : S \mapsto \mathbb{R} \tag{1}$$

This paper tries to give some guidelines as to how to find a mapping which could result in good ANN behaviour, namely quick learning, good training and generalization errors, reasonable ANN size.

2 THE FEEDFORWARD ARTIFICIAL NEURAL NETWORK

The ANN can be formally described in many different ways, *e.g.* as a signal flow graph (2), a Petri net (3, 4), a functional graph (5), an attributed graph (6). ANN is an attributed graph $(U, H, \lambda, \alpha, \beta)$ where U is a set of neurons, H is a set of arcs depicting synapses that connect neurons, λ is a function labelling neurons, α a function which attributes neurons with activation functions, and β an attribute function which ascribes weight values to all the synapses.

A single neuron computes its internal activation v_j as a weighted sum

$$v_j = \sum_i w_{ji} y_i \tag{2}$$

where y_i is the output of neuron u_i connected with u_j by way of a synapse with weight e_{ji}. The neuron output value is computed by means of an activation function $\varphi(\cdot)$

$$y_j = \varphi(v_j) \tag{3}$$

which is nonlinear, *e.g.* a sigmoidal

$$\varphi(v) = \frac{1}{1 + \exp(-v)} \tag{4}$$

In a feed forward network neurons are divided into layers: input layer onto which input patterns are mapped, output layer which gives the result, and additionally some hidden layers. There can be no cycles in the graph.

During the learning phase, examples given as *(input pattern, desired answer)* are processed: the result for a given pattern is computed and then compared with the desired answer by means of a cost function E

$$E(n) = \sum_j e_j^2(n) = \sum_j (d_j(n) - y_j(n))^2 \tag{5}$$

where n is the learning step, and j is the index which spans all the output neurons. Then the synapse weights, which are ANN's free parameters, are modified using the delta rule so as to minimize the cost function. In case of an ANN with a single hidden layer

$$w_{kj}(n+1) = w_{kj} - \eta \frac{\partial E}{\partial w_{kj}(n)} = w_{kj}(n) + \eta(d_k(n) - y_k(n))y_j(n) \tag{6}$$

$$w_{ji}(n+1) = w_{ji} - \eta \frac{\partial E}{\partial w_{ji}(n)} = w_{ji}(n) + \eta\varphi'(v_j)\sum_k (d_k(n) - y_k(n))\varphi'(v_k)y_i(n) \tag{7}$$

3 INPUT DATA REPRESENTATION

Some goals must be met by the learning phase. First, a sufficiently small value of the cost function during the training has to be reached. Then, the net must generalize well, that is it has to compute correct answers for input patterns which were not included in the training data. The number of training examples, N, for the ANN to generalize well must satisfy the condition that (2, 7)

$$N > W/\epsilon \tag{8}$$

where W is the number of weights, and ϵ is the accepted error rate. The ANN should be of a reasonable size, both to achieve good generalization (for a given number of training examples), and assure that the learning time is not too long.

In a symbolic problem a mapping which represents symbols as number vectors of a given size has to be found. Several approaches are possible, some widely used ('1–out–of–n'), some proposed here (cubic, correlation minimization).

3.1 1–out–of–n or "unary" method

This is the most natural. A symbol $s^j \in S$, where S is of cardinality N, is represented with a binary valued vector $x^j = [x_1, \ldots, x_n]^T$ defined as

$$x_i = \begin{cases} 1, & i = j \\ 0, & y \neq j \end{cases} \tag{9}$$

Such representation is easy to compute, vectors for different symbols are orthogonal which speeds up learning, high input layer dimension gives greater probability that the training examples will be separable. On the other hand the resulting net is very big requiring long learning time and many training examples are needed for the sake of good generalization.

3.2 Binary

This is the most condensed. Each symbol $s^j \in S$ is represented as a binary number, thus requiring input layer dimension of $\lceil log_2 N \rceil$. There are less synapses, and separability of patterns is greatly hindered. This method is unable to give low training and generalization errors, and thus is rarely used.

3.3 Cubic representation

In this method symbols are represented as p dimensional, $\lceil log_2 N \rceil < p < N$, vectors x^i distributed over a cube I^p in such a way that among all possible N element subsets of $\{0, 1\}^p$, the expected value $E[H(x^i, x^j)]$ of the Hamming distance

$$H(x, y) = \sum |x_i - y_i| \tag{10}$$

is maximized, while the variance is minimized.

It is a method to be used when no information about the structure of the problem at hand is known, and as little as possible should be introduced. Therefore, the symbols represented should easily be distinguished from each other in a space of dimension p, smaller than N, thus resulting in a smaller net, shorter training time and better generalization. The drawback is that the representation for a given size has to be found using a sequential algorithm, which might require some time

3.4 Correlation minimization

In this method the symbols in S are represented with p element vectors, $\lceil log_2 N \rceil < p < N$, such that the expected value of correlation between any two vectors is minimized. This proposition stems from the fact that during learning the effect of one input pattern on weight changes resulting from other patterns can be minimized. Therefore, learning can be quicker.

Representation for a given set of symbols can be found not only with a sequential algorithm, but also using a specially designed dedicated ANN. It is an ANN with one hidden layer of p neurons, and input and output layers of N neurons, which tries to accomplish an auto association of symbols represented with an '1–out–of–n' type representation. The ANN cost function is modified

$$E(w(t)) = E_a(w(t)) + E_b(w(t)) + E_c(w(t)) \quad (11)$$

$$E_a(w(t)) = \frac{1}{2}\sum_{k=1}^{n}(d_k(t) - y_k^{out}(t))^2 \quad (12)$$

$$E_b(w(t)) = \frac{1}{2}\left(\sum_{j=1}^{l} y_j^{hid}(t) y_j^{hid}(t-1)\right)^2 \quad (13)$$

$$E_c(w(t)) = \frac{1}{2}\left(l - \sum_{j=1}^{l} y_j^{hid}(t) y_j^{hid}(t)\right)^2 \quad (14)$$

The weight update rules that follow, are similar to the delta rule. As representations that are sought, activations of the hidden layer are taken. Provided that learning is of pattern–by–pattern type, and examples are given in a random sequence, this algorithm gives results that are superior to those found by the sequential algorithm, it is found much quicker, and provides representations of higher dimensions.

3.5 Correlation minimization exploiting problem structure

If the input patterns can be divided into sub-patterns, and one with greatest influence on output can be pinpointed, then a correlation minimization representation which exploits the problem structure can be found. A dedicated network is built, but now it has to associate single sub-patterns with the desired answer for the whole pattern. A subset of the original training set can be used for this purpose.

This method incorporates all the virtues of standard correlation minimization, but additionally it builds some prior problem specific knowledge into the ANN structure. If it is used, vectors representing different symbols are still easily distinguished from each other, but at the same time those which give similar results in the problem are given representations which are more nearby than other vectors.

4 COMPUTER EXPERIMENT AND DISCUSSION

To compare results when different representations are used, a computer experiment was performed. The problem is the phonological transformation, similar to that of NETtalk (8). The task is to translate a given Polish language text text into a series of phonemes representing the pronunciation. It is a complicated task because of the highly contextual input information that has to be resolved. In figure 1 results are given for different representations. It can be easily seen that it is possible to build a representation of the symbolic data which results in smaller net size but giving validation error comparable to full size unary rep. The best are the correlation minimization methods especially the one taking advantage of a limited insight to the problem structure. Such results are highly problem dependent, but it seems that a little time spent on finding a depiction of symbolic data can pay off in terms of shortened learning time, better generalization, reduced memory re

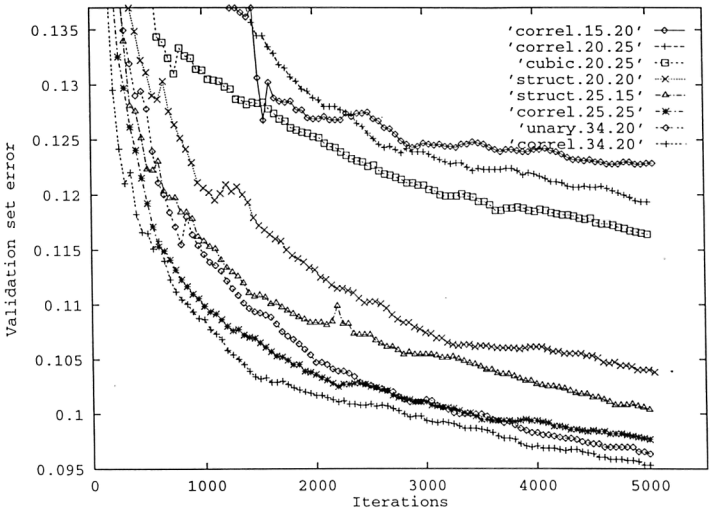

Figure 1: Simulation results using different representations. First number is the size of single letter representation, second the number of hidden units.

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GESAMAC SHARED COST ACTION: LEVEL E/G TEST CASE

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1 FRAMEWORK

The project GESAMAC is a shared cost action (FI4W/CT95/0017) defined into the framework of the IV RTD EC Program in the field of the Programme on Nuclear Fission Safety in the area of Radioactive Waste Management and disposal and decommissioning. The aim of the project is *«to tackle areas of uncertainty, and to develop some conceptual, methodological and computational tools which can be of use in actual safety analysis case studies»*[1]. GESAMAC is a three-year project (1995-1998) with four organisations involved: the EC-JRC-EI of Ispra (Italy), The University of Bath (UK), the University of Stockholm (Sweden) and the CIEMAT-IMA (Spain) which carries on the co-ordination of the Project. Each of the partners has specific points of concern within the project defined by four different work packages (WP): WP1: Geosphere modelling (Spain); WP2: Sensitivity Analysis (Italy); WP3: Uncertainty Analysis (UK), and WP4: Parallel Monte Carlo Driver development (Sweden). At the end of the first project year, it was deemed useful to define a test case for the methodologies and tools in use. This presentation aims to summarise this test case named Level E/G.

2 THE LEVEL E/G TEST CASE

2.1 Objectives

The purpose of GESAMAC is to suggest conceptual and computational methodological improvement (as from the title of the project). The main objective of the Level E/G test case is to promote the collaboration and exchange of knowledge between the different teams involved in the project [2]. In particular, the proposed exercise will

1. test individual methodologies and tools developed (or used) by each team,
2. establish the links between the four 'work packages' defined in GESAMAC,
3. perform a first global trial of the different areas of concern of the project.

2.2 General considerations

An important premise of the disposal system addressed in GESAMAC Level E/G test case, is that it is a generic one where all the data used are synthetic starting from the base case (the PSACOIN Level E).

PSACOIN Level E from PSAG U.G. (OECD/NEA) [3] was taken as a reference since it is a very well documented test case, focuses on the geosphere transport model and has an analytical solution for the transport equation and because it was familiar for most of the partners of the GESAMAC Project. Therefore, the original Level E specifications have been retained, while incorporating other chemical and different structural assumptions and scenarios.

The PSACOIN Level E has been taken as the 'central case' or 'reference case' or 'normal evolution scenario'. It consists in an hypothetical radioactive waste disposal system represented by three coupled sub-models: a near-field, a far-field and a biosphere. The repository itself is represented without any consideration of spatial structure or chemical complexities. The inventory consists in four representative radionuclides: the I-129 and the decay chain Np-237, U-233 and Th-229. After an initial containment time for the wastes, they are leached from the vault with a constant fractional rate. Released radionuclides enter into a geosphere represented by two layers with different physico chemicals properties, where they are transported through (1D diffusive/advective transport equation). Radionuclides leaving the geosphere enter a stream from which the critical group obtains drinking water. The doses received depend on the ratio of the drinking water consumption and the stream flow rate.

3 GENERAL APPROACH TO THE TEST CASE

For the purpose of the current test case, additional components were required: alternative scenarios and alternative structural assumptions. In a first step, three macro-scenarios [4] were selected: a) Geological Scenarios; b) Climatic Evolution Scenarios, and 3) Human Activities Scenarios. In a second step, several micro-scenarios were defined for each one of the three general categories above mentioned. Each micro-scenario was associated with different structural assumptions and/or parameters and/or processes. However it could be possible from the structural

and conceptual points of view, to find out similar configurations to some of the micro-scenarios initially established. In such a case they were grouped in a unique scenario. Moreover, each micro-scenario has associated a probability of occurrence, taking into account that the total probability of the scenarios considered must be one.

1. Geological Scenarios: possible changes in the system evolution related with geological processes or phenomena as a result of the local/regional tectonic activity. Three micro-scenarios were distinguished:

G1. Fault passing through the vault (direct pathway to the biosphere)
G2. Fault passing some meters away from the vault (total travel time reduced)
G3. Fault passing far away from the repository (induced changes into the physico-chemical environment)

2. Climatic Evolution Scenarios: The long time periods covered allow changes in the climate environment of the system. The following micro-scenarios were selected:

C1. Fast pathway from the vault to the biosphere.
C2. Glacial Retreat. Ground water flow direction is upwards.
C3. Glacial Advance. Darcy velocities increase with a downwards flow direction

3. Human Activities Scenarios: They refer to the induced changes (direct or not) into the system associated with anthropogenic activities.

H1. Direct human intrusion scenario,
H2. Disposal errors; deficiencies in construction, disposal, operation, etc.
H3. Human intrusion bypassing some barriers
H4. Anthropogenic induced changes on the environment

After the combining process a final list of scenarios was established. The probabilities assigned to each scenario are speculative and synthetic (See table below).

ID.	Scenario	Group	Prob.
FP	FAST PATHWAY TO THE BIOSPHERE	G1 C1 H3	0,1
AG	ADDITIONAL GEOSPHERE LAYER	G2 C2	0,07
GA	GLACIAL ADVANCE	C3	0,2
HDE	HUMAN DISPOSAL ERRORS	H2	0.3
NG	NO GEOSPHERE	H1	0.3
EIC	ENVIRONMENTAL INDUCED CHANGES	H4 G3	0,03

Each scenario is associated with particular structural assumptions: number of geosphere layers, hidrogeological properties, geochemical process, etc. Their combination defines alternative conceptual model for the disposal system.

The project intends to use the geosphere model to study and perform a fully quantitative synthesis of all sources of uncertainty (scenario, structural, parametric and predictive) and, where it applies, the variance-decomposition methods in sensitivity analysis.

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MANAGING THE TYRANNY OF PARAMETERS IN MATHEMATICAL MODELING

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The models of various physical phenomena and their resultant mathematical structure often contain many input variables. In this paper, we will introduce a family of multivariate approximation schemes to capture the input-output relationships of high dimensional physical systems (i.e., those with many input variables). A systematic input-output mapping procedure is prescribed to reveal the hierarchy of correlated effects of the input variables. Without any evident simplification, such an input-output mapping would be NP-complete with computational complexity scaling as s^n where s is the number of sample values of the input in each dimension. The high dimensional model representations (HDMR) are capable of achieving a dramatic reduction in this scaling to now being just polynomic in n when only low order correlated effects of the inputs act to influence the output. The HDMR concept rests on expressing a multivariate physical output function as a superposition of functions over the low order correlated variables. The output function in $n \gg 1$ dimensions often may be accurately represented by a special superposition of low dimensional sub-volumes up to dimension $\ell \ll n$. The limiting form of the representation is captured in a theorem of Kolmogorov, which states that every multivariate function can be written as an additive superposition of appropriate functions of a single variable. The HDMR technique makes the ansatz that high order correlated effects of the inputs are expected to have a negligible impact on the output. Substantial evidence exists to support the validity of this conjecture, including from multivariate statistical analysis and the familiar many body expansion in physics where rarely are interaction terms involving more than two or three bodies significant. The HDMR technique builds on these observations to present a family of compact representations of the system output(s) as an exact hierarchical sequence of variable correlations. The notion of correlation used here goes beyond statistics to include variable cooperativity induced by the physical system structure and dynamics. Each hierarchical term of the HDMR expansion is obtained by applying a suitable projection operator to the output function and each of the terms are orthogonal to each other with respect to an appropriate inner product. A family of HDMRs may be generated with distinct characteristics by different choices of the projection operators. One particular member of this family is the ANOVA expansion used in statistics. Computationally very efficient HDMR s may be generated for a variety of modelling and analysis applications, including the creation of high speed fully equivalent operational models to replace the original model. Besides the computational advantages of HDMR expansions, the hierarchy of identified correlation functions can provide valuable physical insight into the model structure. The notion of a model in this paper also includes input-output relationships in the laboratory. Selected applications of HDMR and a discussion of its general utility are presented along with some future perspectives.

REGRESSION ANALYSIS AND DYNAMIC BUILDINGS ENERGY MODELS

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1 INTRODUCTION

It is only recently that the analysis of the validity and the reliability of models outputs is being undertaken for buildings energy models. Within the context of collaborations with Electricité de France (F), we have performed both sensitivity and uncertainty analyses of dynamic models ([1], [2], [3]).

We are now investigating response surface methodology involving regression analysis and design of experiment, as an alternate technique for the analysis of dynamic models based on large set of parameters. We aim to substitute to the analysed model a low order polynomial metamodel of the only few prominent parameters (often designated as factors). This metamodel can then be used to perform either uncertainty analysis or optimization.

2. RESPONSE SURFACE METHODOLOGY

In a pilot phase, parameter screening techniques should be used prior to regression analysis, in order to determine the few most prominent parameters which should be retained for the computation of the metamodel. Several techniques are used in building thermal analysis; De Wit [1] used sequential bifurcation meanwhile we used group screening [3] and exact differential technique [4].

The regression metamodels used are approximation of model output. Because the analysed model is a dynamic one, metamodel coefficients are time-varying. Model output, say y, is then re-written as follows

$$y(t) = \beta_0(t) + \sum_{j=1}^{k} \beta_j(t) x_j + \sum_{j=1}^{k-1} \sum_{g=j+1}^{k} \beta_{jg}(t) x_j x_g + \sum_{j=1}^{k} \beta_{jj}(t) x_j^2 + \varepsilon(t) \ , \qquad (1)$$

where k is the number of selected model parameter, β are the metamodel coefficients and x_i the parameters values in combination i.

At each time step, the regression coefficients are fitted using ordinary least squares criterion. The « experimental » data used are generated by model simulation and the values taken by the analysed factors are chosen in agreement either with a Doelhert design [5], which guarantees a good exploration of the analysed domain of variation of the factors, or with a Rechtschaffner design [6], which takes account of all first-order interactions and main effects.

The choice of the order of the metamodel is a non-trivial stage. The proposed methodology is as follows :

(i) Start with a first-order metamodel dealing only with the main effects ;
(ii) Continue with a higher-order metamodel dealing with both first-order interactions and main effects ;
(iii) Finally, investigate a higher-order metamodel dealing with quadratic, interactions, first-order interactions and main effects ;

For each stage, we use a Student test and a Pareto (ANOVA like) test to keep only significant effects.

The next stage in Response Surface Methodology deals with the validation of the metamodel. One reliable technique consists on verifying that the actual model output at a given combination is close enough to the metamodel output since this combination has not been used yet for fitting the coefficients. Kleijnen proposes a cross-validation technique for which no new simulation is needed [7].

2 THE MODEL ANALYSED

The analysed model is the thermal model of the Etna test-cells [8], a real-size experimental building developed on the CLIM2000 software [9]. The model output analysed is the prediction of indoor air temperature.

3 RESULTS

As part of a pilot phase, an exact differential screening was performed on the 390 model parameters; at a given time step, only 9 were found very influent : the floor concrete thickness, surface, specific heat and specific capacity; surface heat exchange coefficient for the floor, both indoor and outdoor surfaces of north wall, and inner surface of south glazing and the latter surface [3]. By using as coefficient β_0 the base case model output and as coefficient β_j the computed first-order derivative for the j^{th} parameter, we derived the following metamodel

$$y(t) = \beta_0(t) + \sum_{j=1}^{k} \beta_j(t) x_j \tag{2}$$

for these prominent parameters.

In order to validate this metamodel, we used a Rechtschaffner design to test whether the error between the output of (2) and the actual model response surface is smaller than 0,1°C (this error is small enough for the temperature analysed in our study). It was found that this criterion was always satisfied apart for a period of 10 hours starting when the heater was switched on. Consequently, for this period, a first-order metamodel is not sufficient to accurately describe the response surface. Taking account of higher order interactions is then necessary.

Using the model run derived with combinations of parameters of a second order Doelhert design (91 runs for 9 parameters), an all interaction and main effects metamodel

$$y(t) = \beta_0(t) + \sum_{j=1}^{9} \beta_j(t) x_j + \sum_{j=1}^{8} \sum_{g=j+1}^{9} \beta_{jg}(t) x_j x_g \tag{3}$$

was identified. Then we used runs from the previous Rechtschaffner design for validation. The error between the identified metamodel and the actual model output was larger than 0,1°C (actually 0.14°C). The metamodel was then judged not valid.

Increasing metamodel order, an all quadratic, interaction and main effects metamodel

$$y(t) = \beta_0(t) + \sum_{j=1}^{9} \beta_j(t) x_j + \sum_{j=1}^{8} \sum_{g=j+1}^{9} \beta_{jg}(t) x_j x_g + \sum_{j=1}^{9} \beta_{jj}(t) x_j^2 \tag{4}$$

was identified. By using a cross-validation technique, we checked that the error between the identified metamodel and the actual model output was smaller than 0,1°C (actually 0,004°C). The metamodel was then judged valid. A student test indicated that all identified coefficients were significant at least once during the analysed period. The Pareto test indicates however that they are the only 9 main effects and the quadratic effect of the floor heat exchange coefficient. The retained metamodel is the following

$$y(t) = \beta_0(t) + \sum_{j=1}^{9} \beta_j(t) x_j + \beta_{11}(t) x_1^2 \tag{5}$$

where x_1 indicates the values of the floor heat exchange coefficient.

4 CONCLUSION

Regression analyses indicates that the analysed model has only few non-linear parameter effect. In addition, the latter is connected with the most influent parameter. Thus, it is believed that non-linearity are likely to be significant for parameter with large effect only.

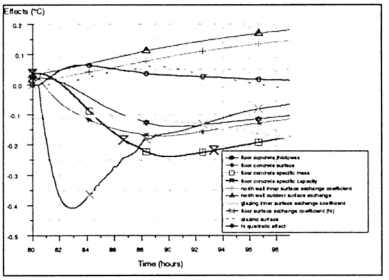

Figure 1: The retained effects

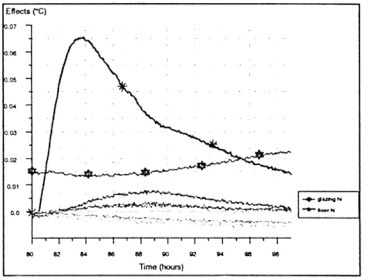

Figure 2: All quadratic effects

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UNCERTAINTY IMPORTANCE OF CORRELATED VARIABLES IN THE PROBABILISTIC PERFORMANCE ASSESSMENT OF A NUCLEAR WASTE REPOSITORY

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1 INTRODUCTION

The performance assessment of potential nuclear waste repositories in geological media, such as Yucca Mountain, U.S.A. [1], involves the application of a sequence of computer models incorporating the complex processes of multi-phase flow and radioactive contaminant transport. There are about four hundred stochastically described inputs to these process models and typically one hundred Monte Carlo simulations are performed to quantify the uncertainty in the predictions of performance measures such as the total peak dose at 1,000,000 years. Uncertainty importance analysis is conducted to identify the dominant input variables responsible for the uncertainty of the output. This analysis involves fitting a response surface to the output function and using the response surface for further importance ranking study.

The variance of the output function is taken as an effective scalar measure of the uncertainty in the output. In probabilistic methodology, importance measure is expressed in terms of "R square", which is the fraction of the variance in the output attributable to the particular input variable. Any importance measure must be in compliance with this notion of "R square". Among the linear-regression-based analysis tools, standardized regression coefficients (SRC), partial correlation coefficients (PCC) and step-wise regression have been widely applied in the performance assessment of other potential nuclear waste repositories, such as the Waste Isolation Pilot Plant (WIPP) site [2] in the U.S.A.

The computational strategy adopted for the performance assessment of the Yucca Mountain site results in strongly correlated input variables. The uncertainty importance study is therefore rendered more difficult. References to the case of correlated input are few and vague in the currently available scientific literature [3]. This study is therefore directed at identifying the correct procedures for uncertainty importance study for correlated input variables in linear-regression-based methodology. From among the four hundred inputs, twenty-five variables have been selected by expert judgement for further importance study. The tools of step-wise regression and partial correlation have been applied for this analysis. Different aspects of step-wise regression viz., the order of entry of the variables, the SRCs and the successive increments in R^2, are used for importance ranking. The PCCs computed on the basis of all 25 variables are also used for ranking. However, the results obtained here show that the different criteria in step-wise regression do not agree among themselves. They are also in disagreement with those from PCC. The results of the step-wise regression also show that the variable importance gets re-shuffled as more variables enter (or leave) the model. These difficulties are identified as symptoms or manifestations of the input correlations.

2 UNCORRELATED INPUT: ANALYTICAL DERIVATIONS

To comprehend the complications due to correlations in perspective, a clearer understanding of the uncorrelated input case is needed. So, the analytical solutions for the uncertainty importance measures employed

in step-wise regression and in partial correlation coefficients for the special case of independent input variables are derived and presented. These analytical solutions clarify why the different criteria lead to the same importance ranking of the input variables in the ideal case of independent input. Many of the applications in the field such as at the WIPP site, are in conformity with these theoretical cases, suggesting that the solutions can be extended to the cases of weak correlations also. For these cases, the derivations also show that the importance ranking by sample correlation coefficients would be in agreement with those from the sophisticated tools such as the step-wise regression and partial correlation. The WIPP example [2] demonstrates this aspect also.

As one example of these derivations, the relation between the PCC and the sample correlation coefficient is presented below:

$$PCC_j^2 = \left[1 - \frac{1}{1 + \{ r_j^2 / (1 - R^2) \}} \right] \tag{1}$$

where PCC_j and r_j denote (respectively) the PCC and the sample correlation coefficient for the j th input variable with respect to the output variable. Also, R^2 denotes the coefficient of determination of the linear regression model (with j th input variable included). Equation 1 brings out that the importance ranking by PCC and sample correlation coefficient would be identical for the case of uncorrelated input.

3 STANDARDIZED REGRESSION COEFFICIENTS

It is shown for the case of independent input that the square of the standardized regression coefficient can be interpreted as fractional variance, a fundamental importance measure. Unfortunately, this interpretation becomes invalid in the presence of input correlations. Thus the SRC should not be used as a measure of importance for the correlated input.

4 PARTIAL CORRELATION COEFFICIENTS

In the sensitivity analysis literature [2], PCC has been interpreted to indicate the strength of a linear relationship (correlation) between an input variable and the output variable, after eliminating the correlation of the other input variables. This suggests that PCC can be a robust importance measure for use in correlated input cases. To clarify this aspect, another interpretation of the PCC implied in multiple linear regression analysis has been invoked. The square of a PCC gives the increase in R^2, when a new variable is added, as a fraction of the currently unexplained variance in the model.

Consider a multiple regression model, whose coefficient of determination is R^2. If the j th input variable is brought into the regression model, the gain in R^2, denoted as $\left(R^2_{gain}\right)_j$, is given by:

$$\left(R^2_{gain}\right)_j = PCC_j^2 * (1 - R^2) \tag{2}$$

The PCC can also be related to the reduction in R^2, when a variable is dropped from a model. From an existing regression model with a coefficient of determination R^2, if the k th input variable is dropped, the reduction in R^2, denoted by $\left(R^2_{loss}\right)_k$, is given by:

$$\left(R^2_{loss}\right)_k = \frac{(1 - R^2)}{\left(\frac{1}{PCC_k^2} - 1\right)} \tag{3}$$

These relationships between the PCC and the R^2-changes remain valid whether the input variables are uncorrelated or correlated. Thus PCC is an index of the fractional variance of that input variable, a fundamental importance measure. It has been shown that the PCCs provide a robust importance measure in linear models with strongly correlated input, where sometimes, the variance-partitioning schemes [4] are hard to implement due to the unduly large regression coefficients.

5 IMPLEMENTATION STRATEGY

As a result of the input correlations, the importance rankings depend upon the variables present in the regression model. Therefore the suggested strategy for using PCC is as follows. Build an optimal regression model, striking a parsimonious compromise between model complexity and its goodness-of-fit. The variables in this model constitute the best sub-set of input variables for the number of variables selected. This is typically done by a step-wise regression procedure. This procedure uses PCC to add or drop a variable , which is a valid index of R^2-changes, in the presence of strong input correlations. But the usual criteria for importance in step-wise regression, namely, the order of entry of variables, or SRCs, or the increment in R^2 when a variable enters, are all invalid indices and should be ignored. When the optimal model is reached, the PCCs of the variables in the final model provide the correct importance ranking. It is to be recognized that an optimal model becomes a pre-requisite for correct importance ranking. This difficulty does not exist for the case of independent input, where the rankings are unique and merely depend upon the absolute values of the sample correlation coefficients!

6 CONCLUSION

A methodology for uncertainty importance ranking of correlated stochastic inputs in Monte Carlo Simulation is presented here. An interpretation of the partial correlation coefficients, as implicit indexes of the gains or losses in the coefficient of determination (R^2) of the multiple linear regression model, when variables are admitted into or dropped from the model, has been highlighted. This interpretation, which remains valid in the presence of strong correlation of input variables, clarifies the validity and robustness of the partial correlation coefficients as uncertainty importance measures. The importance rankings of input variables get re-shuffled as more variables enter or leave the model. In view of this, an optimal regression model becomes a pre-requisite for importance ranking, unlike in the case of uncorrelated input; and the partial correlation coefficients in this model provide the correct importance ranking. Also, analytical derivations for uncertainty importance measures commonly in use have been obtained for the idealized case of uncorrelated inputs. For this case, it has been shown that sample correlation coefficients provide the correct importance ranking and that the other sophisticated tools in use correspond to a more complicated but equivalent implementation of this simple measure.

7 ACKNOWLEDGMENTS

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FREQUENCY DOMAIN SENSITIVITY OF BUILDINGS ENERGY MODELS

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1 INTRODUCTION

Within the context of collaborations with Electricité de France (F) and the Building Research Establishment (UK), the LETIEF laboratory aims to develop techniques for analysing the validity and the reliability of models outputs for buildings energy dynamic models (ref. 1-2).

Since 1992, we are developing and testing tools for diagnosing modelling errors by comparing model and experimental data. In order to analyse dynamic behaviours, the frequency response to actual excitation is used as model output. This « model » frequency response is then compared to the one derived for the actual system by parametric identification (ref. 3). Comparing transfer functions reveals a powerful tool capable of disaggregating the actual effects of several inputs, at different time-scales.

We are now interested in the computation of the sensitivity of the « model » transfer function to model parameters, as we believe that this can help giving a comprehensive analysis of the connection between the physical phenomena described in the model and its dynamic behaviour. If the model were valid, such a work could lead to a better understanding of the connection between the actual physical phenomenon and the actual behaviour of the system analysed.

2 ADJOINT METHOD FOR SENSITIVITY COMPUTATION

Because the systems modelled often involve a large number of parameters, the computation of the sensitivity of model output to model parameters using a direct perturbation approach is not feasible. Contrariwise, the adjoint (or transpose) method is more adapted as it only requires the resolution of a set of algebraic equations with the same complexity as the original system, irrespective of the number of parameters analysed (ref. 4-6). According to (ref. 6), this is summarised as follows:

Consider a system of linear equations

$$T \cdot X = W , \tag{1}$$

where T and W may be real or complex and depend on some parameters h_i. The solution of (1) is written formally as follows:

$$X = T^{-1} \cdot W \tag{2}$$

Suppose, as it is usually the case, that one is interested in a single output f, a combination of the component of X

$$\phi = d^t \cdot X \tag{3}$$

The desired sensitivity can then be obtained by the following

$$\frac{\partial \phi}{\partial h_i} = \left(X^a\right)^t \frac{\partial T}{\partial h_i} X - \left(X^a\right)^t \frac{\partial W}{\partial h_i} \tag{4}$$

In (4), the vector X is obtained prior to sensitivity computation and the vectors

$$\partial T/\partial h_i \text{ and } \partial W/\partial h_i$$

are obtained through formal derivation. Relation (4) exhibits a new vector X^a termed adjoint vector; X^a is the solution of

$$T^t \cdot X^a = -d \tag{5}$$

Finally, since a factorization of the original system automatically factorizes the adjoint system, the sensitivity of a model output to all parameters is available at the sole extra cost of one single substitution into the adjoint system.

3 THE MODEL ANALYSED

The model analysed is the thermal physical model of a real size experimental building [5] developed on CLIM2000 software. The model uses 201 constant parameters. CLIM 2000 is a graphical pre-processor designed at the Research Centre of EDF. The algebro-differential equations thus obtained by assembling elementary models are then solved by ESACAP software, which is an electrical network analysis program developed by StanSim Research Ltd. The ESACAP software is capable of handling variable in the Laplace domain (and also in the frequency domain) and hence furnishes the « model » transfer function through classical circuit relationships. We are interested in the « model » frequency response to the input « heating operation ».

Figure 1 shows the gain and the angle of the analysed model output, for frequencies ranging from $10^{-8}hz$ to $1hz$. At $f=10^{-8}hz$, the gain is constant and the angle is null ; the behaviour can be regarded as static. At $f=1hz$, the gain is totally dampened and the angle equals -90*degrees (°);* the output variations are totally filtered. As expected, the indoor temperature response to « heater operation » excitation can be regarded as a « low-pass filter ». The odd angle shape exhibit a complex dynamic behaviour.

4 THE COMPUTED SENSITIVITIES

The adjoint method is applied to the previous model. At each frequency, a Lenth test is used to identify the most influent parameters (ref. 7). Only 15% of the whole parameters set are judged influent at least once over the analysis frequency range.

The analysis of the sensitivities derived helps the identification of three frequency bands where sensitivity values are similar. These bands are regarded as representative of a « slow dynamics » behaviour for $f=[10^{-8}hz, 3\cdot10^{-7}hz]$, a « medium range dynamics » for $f=[3\cdot10^{-7}hz, 10^{-3}hz]$, and a « fast dynamics » for $f=[10^{-3}hz, 1hz]$.

As expected, « slow » dynamics, are found to be sensitive to both convective and conduction phenomena. It is the most conductive walls (the less isolated) which appear to be the most influent.

The « rapid » dynamics are sensitive to indoor air-wall convective exchanges and indoor volume specific heat.

The « medium-range » dynamics involve a more complex combination of conduction and heat accumulation phenomena. Figure 2 contains the sensitivity to the floor components parameters. It shows that the « medium-range » gain is sensitive to heat accumulation phenomena whereas the angle is also sensitive to convective and conductive heat exchange near the inner floor surface.

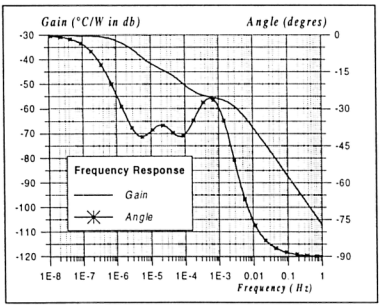

Figure 1: Model output.

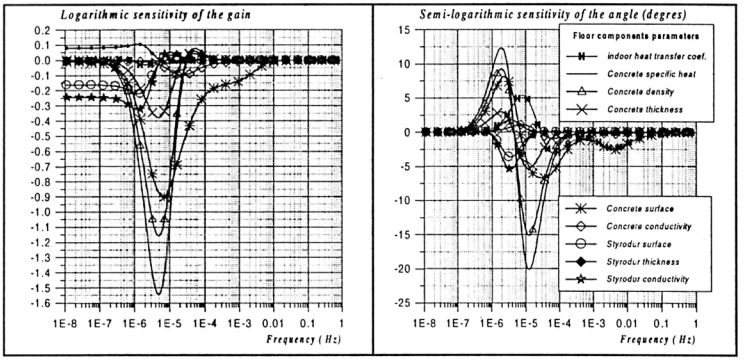

Figure 2: Frequency domain sensitivity to parameters of floor components.

5 CONCLUSION

The derivation of the frequency domain sensitivities offers new prospects in model validation. The next step is the computation of uncertainty bands in the frequency domain. Such an uncertainty analysis can help identifying the time-scales where model dynamics are not reliable. Since the frequency domain sensitivities are available at low computational cost, one can implement miminization routines in order to test whether a discrepancy between model output and any « reference » output can be explained by errors or discrepancies in some model parameters. Such results offer new prospects in model validation.

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UNCERTAINTY ANALYSIS OF A FIXED-BED GAS-SOLID TSA

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1 INTRODUCTION

In this study the analysis of the effects of uncertainties on model outputs is reported for a multicomponent gas-solid TSA fixed-bed adsorber. The uncertainty analysis is carried out applying the first order differential analysis. Despite its simplicity, this analysis is effective in describing the main effects of uncertainties and identifying the most critical aspects, which thwart an *a priori* description of the process under study, and which therefore have to be improved.

2 PROBLEM FORMULATION

The most critical aspects of adsorption models are: adsorption equilibrium and mass and heat transfer between the phases and inside the solid particles. Many improvements have been adopted by many authors in order to obtain a good predictive model: non-isothermal or adiabatic system, axial dispersed plug-flow model for the fluid phase and diffusional model inside the particles with constant or concentration dependent diffusivity (see for instance [1,4]). Among the proposed models, the most complete is that of Farooq *et al.* [1]. Nevertheless, in many cases, such improvements are unfortunately still accompanied by rough thermodynamic descriptions and, also in more complete works, where multicomponent systems with non-linear equilibrium isotherms are considered, the Langmuir isotherm, which offers the easiest description of multicomponent adsorption but obviously not the best one, is mainly used. This could represent a limitation for the reliability of predictions.
In this work we considered a relatively rigorous but sufficiently simple model, describing an industrial gas-solid temperature-swing adsorber of organic compounds; parameters and their variance are supposed to be known. Different kinds of uncertainty are taken into account:

- *Parameter uncertainty*: uncertainty has been considered for equilibrium parameters (a Freundlich isotherm for the single component and the IAS theory for the multicomponent equilibrium has been taken into account), LDF constant rate coefficient, axial dispersion, inlet temperature and concentration.
- *Model uncertainty*: a comparison between thermodynamic descriptions of growing complexity has been performed: linear isotherm, pure Freundlich isotherm without multicomponent effects and Freundlich isotherm for the single component with the IAS theory for the description of multicomponent adsorption. This was carried out always considering the LDF model for transport phenomena, so that a choice among thermodynamic models of different precision can be made. It will be shown that the problem of whether the transport model has to be improved or not has different answers depending on the accuracy of the thermodynamic description.

3 THE MODEL

In our study we referred to an existing industrial plant. The inlet flow-rate consisted of a mixture of three organic compounds (methylene chloride, acetone, methyl alcohol) and damp air; the adsorbed amount of air is negligible and, including water, a four-component adsorption can be considered. In the reference model, the equilibrium is described by means of a Freundlich isotherm with the IAS theory for the description of multicomponent adsorption. The mass transfer is described by means of the LDF model and axial dispersion is neglected. See Ratto et al. [5] for more details.

4 UNCERTAINTY ANALYSIS

Effects of uncertainties on model output are studied by means of a first order differential analysis. The model output considered for the uncertainty analysis is the predicted duration of the process τ, i.e. the time when the outlet concentration of methylene chloride rises above a given value. The reference value τ_r obtained with the reference model without uncertainties is 28800 s. It is supposed that the parameters and their variance are known.

Indicative values for their standard deviation are given in Table 1.
The following parameters were considered for the uncertainty analysis:

- parameters of the Freundlich equilibrium isotherm of the methylene chloride

$$q = F \cdot p^{tF} \tag{1}$$

with the temperature dependence of the equilibrium parameters given by

$$\begin{aligned} \ln F &= \alpha - \beta T \\ t_F &= \gamma + \delta T \end{aligned} \tag{2}$$

- the inlet temperature T_0;
- the inlet concentration of methylene chloride and water (c_0^{meth} and c_0^{water});
- the heat transfer coefficient h;
- the constant Ω in the LDF coefficient calculated neglecting the external film resistance and given by

$$k_{pi} = \frac{\Omega}{3} \cdot \frac{D_i^{eff}}{R_p} \tag{3}$$

Considering the parameters (indicated as x_j) to be uncorrelated, the estimation of the variance and standard deviation of the duration of the process is given by:

$$V(\tau) \approx \sum_{j=1}^{n} \left[\frac{\partial \tau}{\partial x_j} \right]^2 V(x_j) = 224256236\ s^2 \quad \Rightarrow \quad SD(\tau) = 14975\ s \tag{4}$$

The impact of each parameter on the uncertainty of τ is given by

$$\frac{\partial \tau}{\partial x_i} \frac{SD(x_i)}{SD(\tau)} \tag{5}$$

Results are summarised in table 1.

Table 1: Sensitivity and uncertainty analysis.

Parameters x_i	*Estimate*	*SD(x_i)*	*impact*
α	*9.18527*	*0.27556 (±3%)*	*0.44714*
β	*3.7577 10^{-2}*	*1.13 10^{-3} (±3%)*	*-0.54753*
γ	*-6.5861 10^{-2}*	*0.1317 (±200%)*	*-0.26709*
δ	*2.1945 10^{-3}*	*6.6 10^{-4} (±30%)*	*-0.3606*
T_0	*300 K*	*5 K (±1.67%)*	*-0.41495*
c_0^{meth}	*2 10^{-3} kg m^{-3}*	*1 10^{-4} (±5%)*	*-0.03673*
c_0^{water}	*6.8 10^{-3} kg m^{-3}*	*3.39 10^{-3} (±50%)*	*0.04673*
Ω	*14*	*7 (±50%)*	*0.35098*
h	*5 10^{-3} J m^{-2} s^{-1} K^{-1}*	*2.5 10^{-4} (±5%)*	*0.00167*

The impact of the thermodynamic and mass transfer parameters is preponderant with respect to the other parameters. Temperature is also important. The feed temperature is a process parameter and sensitivity to temperature is a typical problem of operation and not of modelling. Therefore, if sensitivity to the temperature is high, the possibility to use a temperature controller should be evaluated.

5 SENSITIVITY OF PREDICTIONS TO MODEL UNCERTAINTY

In this case the uncertainty analysis was performed comparing directly the values of τ obtained using the different models, considering the quantity

$$\left| \frac{\tau - \tau_r}{\tau_r} \right| \tag{6}$$

which corresponds in a certain way to the impact calculated in the previous section. Another two equilibrium models were considered: a single component Freundlich isotherm (without any multicomponent effect) and a linear isotherm. The equilibrium constants Y_i of the linear isotherms were determined as

$$Y_i = \frac{q_{i0}^*}{c_{i0}} \tag{7}$$

where q_{i0}* is the adsorbed quantity in equilibrium with the inlet concentration. A comparison with an axial dispersed model is also performed. Results are summarised in Table 2.

Table 2: Effects of the choice of the model

Different models	τ	$\left\|\frac{\tau-\tau_r}{\tau_r}\right\|$
Reference model	*28800*	*0.0*
Pure Freundlich isotherm	*32400*	*0.125*
Linear isotherm	*15700*	*0.455*
Axial dispersed model	*28700*	*0.00347*

The effect of axial dispersion is very small. Nevertheless, axial dispersion is often considered in dynamic simulation, since it facilitates the numerical computation by eliminating discontinuities in the slope of the concentration profiles.

On the other hand the choice of the equilibrium model strongly affects predictions, with an impact similar to that of the thermodynamic and mass transfer parameters. The linear isotherm, as expected, is compeltely unreliable. More interesting is that there is an appreciable difference between the reference model and the pure Freundlich isotherm. Since the Freundlich (as well as the Langmuir) isotherm, is not the best available equilibrium model, a predictive model might be possible only if a more complex model, even for the single component, was taken into account.

6 DISCUSSION

As in previous works, it comes out that there are two particular aspects to be developed in order to obtain a good predictive model: mass transfer and adsorption equilibrium. Predictions depend very much on the choice of the equilibrium model. Nevertheless, the impact of the uncertainty of thermodynamic parameters is greater than that coming from the different models, therefore a complex and accurate model has no meaning without reliable experimental data, by which parameter uncertainty is reduced.

The numerical simulation being time-consuming, a complication of the model has to be justified with real advantages in the prediction capability. Therefore, if the effects of experimental errors remain preponderant, a complex model would probably be useless. Furthermore the improvement introduced in a complex model must be homogeneous for the different aspects of the described system. In our case a good mass transfer model accompanied by a rough thermodynamic description would not be an optimal choice and a waste of time. In conclusion we can staye that:

1. A predictive model is possible if we simultaneously improve the description of both thermodynamics and kinetics.
2. Parameter uncertainty can seriously affect predictions, therefore a correct mathematical model might not be sufficient, without an accurate experimental analysis.

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SENSITIVITY ANALYSIS AS ACCURACY MEASURE OF A SIMPLIFIED STRONGLY NON-LINEAR THERMAL MODEL USEFUL FOR TRANSFORMERS' RELIABILITY STUDIES

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1 INTRODUCTION

Main factors constraining transformers' thermal loss of life are load and ambient temperature profiles they are subjected to. Provided a suitable transformer thermal model and a loss of life one are chosen, it is possible, from a theoretical point of view, to determined its on-line expected loss of life [1].
However, if the objective is a long term planning, inherent errors of load and ambient temperature profile forecasts (due to any unpredictable increases or decreases in load or ambient temperature), will be greatly amplified by the strongly non-linear nature of the thermal ageing model. Due to the random character of independent constrains, such a purely deterministic approach will lead to reduced reliability results.
Real load and ambient temperature profiles do present a deterministic cyclic component (daily, weekly, monthly, seasonally) to which is superposed a random behaviour; these physical characteristics of the real profiles, impose a probabilistic approach [2, 3] for the study of transformer expected loss of life.
A work has already been presented relative to model's output sensitivity to input functional parameters K and T [4]. Such a study is justified by the variability (both on deterministic and random components) that load and ambient temperature profiles do present under realistic conditions. Usually, model's structural parameters are assumed to be known without error. Some of these parameters are transformer specific ones ($\Delta\Theta_{oR}$, $\Delta\Theta_{ohR}$, R), determined either from tests either from manufacturer catalogue data, and do present some variability for a given transformer rated power, dependent upon manufacturers [5]. Others (n and m) are hard to determine with precision from tests, since they are closely related to transformer cooling conditions and geometry.
The variability that these parameters do present in practice, is the base of this study which objective is, under a reference scenario of functional inputs, to analyse model's output (*LOL*) sensitivity, to model's structural parameters, namely, $\Delta\Theta_{oR}$, $\Delta\Theta_{ohR}$, R, n and m.

2 TRANSFORMER *LOL* MODEL

Transformer thermal characterisation and insulation materials degradation is an old subject of many works. We assumed the standardised models and methodology presented in [1] which terminology is briefly recalled. Figure 1 represents the block diagram including input variables (load **K** and ambient temperature **T**) and output ones (loss of life: **LOL**).

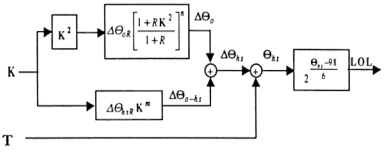


Figure 1 – Block diagram of transformer thermal and loss of life models.

Under steady-state conditions, transformer hot-spot temperature Θ_{hs} [K] is given by:

$$\Theta_{hs} = T + \Delta\Theta_{oR}\left(\frac{K^2R+1}{R+1}\right)^n + \Delta\Theta_{hsR}(K)^m \quad (1)$$

where:

$\Delta\Theta_{oR}$ -Top-oil rise under rated load [K]

$\Delta\Theta_{ohR}$ -Hot-spot rise over ambient temperature at rated load [K].

R - Loss ratio (Load /No-load) at rated load [p.u.]

n - Oil exponent [dimensionless]

m - Hot-spot thermal exponent [dimensionless]

According to [1] the relative ageing rate V [p.u.] is based upon a constant ambient temperature of 20°C, which means a reference hot-spot temperature of 98°C:

$$V = 2^{(\Theta_{hs}-98)/6} \quad (2)$$

To determine LOL over a certain period of temporal variations, and attending to data discrete type, [1] defines:

$$LOL = \frac{1}{J}\sum_{j=1}^{J} V_j \quad (3)$$

with:

V_j - Relative ageing rate of time interval j [p.u.]

j - Number of each time interval

J - Total number of equal time intervals

In fact, (2) corresponds to a deterministic point of view, since it represents an integral of V temporal variation; under a probabilistic formulation, being the statistical distribution stationary, time dependence is eliminated and so $V \equiv LOL$.

3 METHODOLOGY

3.1 Referential Scenario

Figure 1 functional inputs (K, T) are the transformer load and ambient temperature profiles which we will assume can be represented by an additive model of deterministic (d) and random (r) components, of the form:

$$K = K_d + K_r \quad \text{and} \quad T = T_d + T_r \quad (4)$$

In this paper we will consider deterministic component stationary. In fact, this basic representation on functional input profiles will have no influence on structural parameter sensitivity study, since these profiles will remain unchanged along the study.

We considered that both system functional input variables are normally distributed:

$$K \sim N(\mu_K, \sigma_K) \quad \text{and} \quad T \sim N(\mu_T, \sigma_T) \quad (5)$$

where μ_x and σ_x represent the variable two first moments, *expected value* and *standard deviation*, respectively, which values are: $\mu_K = 1 p.u.$, $\sigma_K = 0.1 p.u.$, $\mu_T = 20°C$ and $\sigma_T = 5°C$.

For the reference scenario, structural parameters will be considered as deterministic variables, which values are those proposed by [1]:

$$\Delta\Theta_{oR}=55\ \text{K}, \qquad \Delta\Theta_{hsR}=23\ \text{K}, \qquad R=5, \qquad n=0.8, \qquad m=1.6 \quad (6)$$

3.2 Statistical Scenario

For this scenario, structural parameters will be considered as random variables. Other possible distribution could be envisaged dependent upon the available knowledge of parameters; due to its generality, we will consider structural parameters as random variables normally distributed:

$$\Delta\Theta_{oR} \sim N(\mu_{oil}, \sigma_{oil}),\ \Delta\Theta_{hsR} \sim N(\mu_{hs}, \sigma_{hs}),\ R \sim N(\mu_R, \sigma_R),\ n \sim N(\mu_n, \sigma_n) \quad \text{and} \quad m \sim N(\mu_m, \sigma_m) \quad (7)$$

which first moment values are those of (6) and second moment ones are imposed by physical conditions:

$$\Delta\Theta_{oR},\ \Delta\Theta_{ohR},\ R,\ n,\ m > 0 \quad , \quad n < 1 \quad \text{and} \quad m < 2 \quad (8)$$

3.3 Procedure

Using a Monte Carlo simulation method [6], load and ambient temperature profiles are simulated and, under the referential scenario, output variable two first moments μ_{LOL} and σ_{LOL} are determined.

The model's output sensitivity will be studied separately for each structural parameter. Five more simulations are performed where, one at the time, each structural parameter is considered as a random variable defined on (7), while

he remain four, stay as deterministic ones; like this, one is able to study output sensitivity due to each parameter eparately.

The variability of each parameter was incremented up to the limits imposed by physical conditions (8). This variability :an be measured through the *variation coefficient*, defined as

$$\gamma = \sigma / \mu \tag{9}$$

The output variable sensitivity is measured through the *LOL* variation coefficient, in per unit values based on those)btained under the referential scenario.

$$\gamma_{LOL}[p.u.] = \frac{\gamma_{LOL}}{(\gamma_{LOL})_{\text{Referencial}}} \tag{10}$$

4 SIMULATION RESULTS AND ANALYSIS

4.1 Simulation Parameters

The results presented, were obtained considering a standardised distribution transformer rated 630 kVA, 10 kV / 400 V with copper windings.

Input variables sample length is N= 3 000 and were simulated from a Monte Carlo method [6].

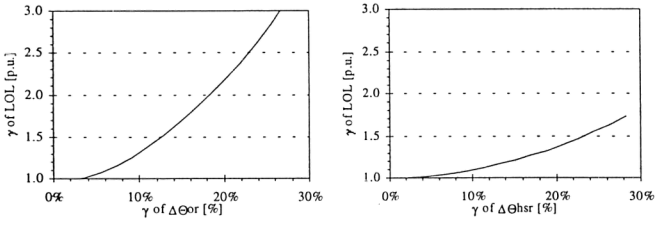
In order to compare, separately, model's sensitivity to each parameters, five set of input data were considered, Table 1:

Table 1 – Structural parameter values

Set	$\Delta\Theta_{oR}$ [°C]	$\Delta\Theta_{hsR}$ [°C]	R [p.u.]	n	m
A	μ=55 and $\sigma \in$ [0; 15]	23	5	0.8	1.6
B	55	μ=23 and $\sigma \in$ [0; 6.5]	5	0.8	1.6
C	55	23	μ=5 and $\sigma \in$ [0; 1.4]	0.8	1.6
D	55	23	5	μ=0.8 and $\sigma \in$ [0; 0.2]	1.6
E	55	23	5	0.8	μ=1.6 and $\sigma \in$ [0; 0.4]

4.2 Results

Simulation results are represented on Figures 2, 3 and 4.



(a) *(b)*

Figure 2 – LOL sensitivity to $\Delta\Theta_{oR}$ *(a)* and $\Delta\Theta_{hsR}$ *(b)* variability

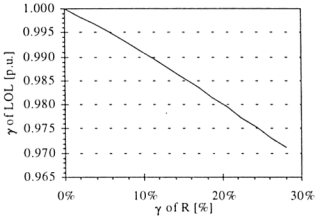
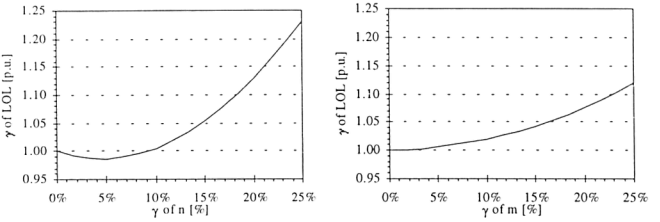


Figure 3 – LOL sensitivity to R variability



(a) *(b)*

Figure 4 – LOL sensitivity to n *(a)* and m *(b)* variability

5 CONCLUSIONS

LOL sensitivity to $\Delta\Theta_{oR}$ and $\Delta\Theta_{hsR}$ parameters' variability is important (Fig. 2). In fact these are the thermal model parameters that represent the transformer's cooling conditions which are fundamental on hot-spot temperature estimation and so loss of life. Results show the importance of standardise these to parameters with variation coefficients below 5% so that LOL sensitivity to them becomes negligible.

Output sensitivity to R parameter's variability is negligible (Fig. 3) since, even with an increase in transformer losses (which would increase LOL), this R ratio stays almost constant. R is a fundamental parameter to optimise transformer efficiency as a function of load variability and losses economic value but its importance is reduced on hot-spot temperature estimation, at least assuming [1] thermal model.

Sensitivity to n and m parameter is an important subject since many discussions can be found on recent literature about these two parameters. Its importance can be considered reduced compared to $\Delta\Theta_{oR}$ and $\Delta\Theta_{hsR}$ one.

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INVESTIGATION OF MODEL AND PARAMETER UNCERTAINTY IN WATER QUALITY MODELS USING A RANDOM WALK METHOD

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ɜSTRACT

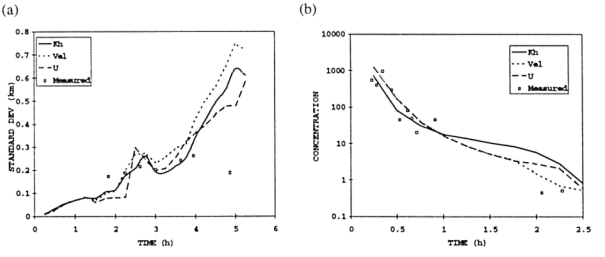
ıathematical model to predict the effect of chemical spills on the Forth estuary in Scotland has been in use for many years. The ɗel, based on the random walk method, predicts chemical concentrations in the estuary waters and estimates the elapsed time ʼore the dilution is sufficient to render the spill harmless (making use of a toxicity measure such as the LC50 or a water quality ıdard). The model gives a deterministic result without any estimate of the uncertainty. However field studies have shown that mixing in the estuary varies on a day to day basis and the literature on turbulent diffusion shows that there are different ways to ɗel the mixing process; this paper investigates the uncertainties due to model formulation and parameter variability, and ımates the possible range of estuarine concentrations for a specific spill scenario.

INTRODUCTION

ɛ estuary model is based on a particle tracking random walk method [1] and has been set up for the Forth estuary in Scotland. ɛ model has been calibrated against a range of field data from the estuary [2]. In particular the calibration of mixing in the model s based on comparisons with dye tracer studies of relatively short timescale (6 hours or less), yet the model has been used for ılating the effects that last for several tidal cycles. Two aspects of the uncertainty are considered below; namely the theoretical rmulation used for the mixing and the variability in the measured mixing rates.

THE CHOICE OF MODEL MIXING THEORY

ɛ horizontal mixing can be parameterised in different ways - for example, using a constant mixing coefficient approach [3], a ɑing velocity formulation [4] or a method relating the mixing rate to the tidal current speed [5]. Using these three different ɔroaches the data from a 6 hour dye experiment have been simulated using the random walk model. All of the methods can ɛquately represent the measured dye patch spread and dilution from a 6 hour experiment carried out on 13/7/88. Fig 1 shows the ɱparison of the methods against the measured data on dye patch size and the dye concentration.



g 1: Comparison of predicted and measured values for (a) standard deviation of the horizontal patch size and (b) peak dye concentration.

ɕh of the mixing formulations has been used to simulate the rate of dilution of a chemical spill in the estuary over a ʼiod of four tidal cycles. Fig 2a shows the three different predictions of concentration, which vary by up to a factor of times (at time 20 hours after the spill). By the end of four tides the predictions have converged, because the effluent

has mixed fully across the estuary cross section area. If the safe concentration were as indicated by the dashed line on Fig 2a (0.005 mg l^{-1}) then the modelling estimates that the time required for the concentration to reach the safe level is 10, 22 and 36 hours for the diffusion velocity, constant diffusion and tidal current methods respectively. Thus the uncertainty in the duration of the incident is a factor of 3.6 times. The surface area of the patch with concentrations above the reference level (0.005 mg l^{-1}) is shown on Fig 2b and varies by an order of magnitude between the different theories.

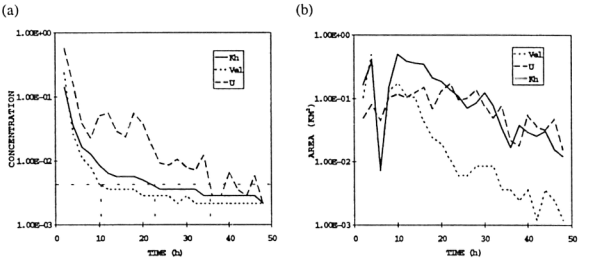


Fig 2: Predicted (a) concentration (mg l^{-1}) and (b) contaminated area (km^2) in the estuary from the three mixing models.

3 VARIABILITY IN MIXING

Repeated studies of dye dispersion in the estuary have shown that there is a significant variability in the transport and dilution from day to day. The data show that the horizontal dispersion coefficient (K_h) varies by a factor of 17 and vertical mixing coeficient (K_z) by a factor of 16. Results from the 7 different dye diffusion experiments are shown in Table 1 below:

Table 1: Dispersion coefficients in the Forth estuary - from dye dispersion experiments.

Date	Time (BST)	Tide	Duration (h)	Horizontal dispersion coeff. (K_h m^2 s^{-1})	Vertical dispersion coefficient (K_z m^2 s^{-1})
7/7/86	0504	Ebb	0.7	-	0.0029
7/7/86	1127	Flood	1.2	-	0.00081
8/7/86	0600	Ebb	1.2	0.18	0.0014
9/7/86	1212	Flood	1.4	0.05	0.00085
21/7/86	1215	High water slack	1.1	0.16	-
13/7/88	1120	Flood/Ebb	5.5	0.75	0.0047
14/7/88	0500	Ebb	3	0.85	0.0003

Repeated measurement of the tidal current at five positions in the estuary over 2 days on spring tides (25/26 June 1979) and 2 days on neap tides (2/3 July 1979) shows a variability of approximately 10 % in the peak current amplitude.

The random walk model has been used to simulate the effect of this variability on the spill dilution; for this simulation the mixing has been simulated using the constant diffusion coefficient model. In the simulation each model particle has been tagged with a horizontal and vertical mixing coefficient and a tidal current factor taken from normal distributions as follows:

$$K_h = K_{hm} + \alpha K_{hs} \qquad K_{hm} = 0.5, \quad K_{hs} = 0.05$$
$$K_z = K_{zm} + \beta K_{zs} \qquad K_{zm} = 0.002, \quad K_{zs} = 0.0005$$
$$C = C_m + \gamma C_s \qquad C_m = 1 \qquad C_s = 0.05$$

where α, β and γ are random numbers from a standard normal distribution, and the subscript 'm' denotes the mean value and the subscript 's' denotes the standard deviation; the uncertainty in the tidal currents is modelled using the factor, C, to multiply the tidal currents. Each particle keeps its values for these three parameters throughout the simulation. At selected times the information for each particle was written to a file together with the particle position information. These data are then analysed using a post-processing program to give concentration information for different ranges of the input parameters. The overall concentration distribution for 12 hours after the spill is shown as a histogram on Figs 3a; the concentration value obtained from a deterministic model run using the mean parameter values is also marked. Concentration ranges from the uncertainty run are given for each half tide of the model run in Table 2 below.

Table 2: Range in the 95 percentile predicted concentration for the spill at half tide intervals

Time (h)	6	12	18	24	30	36
Minimum concentration	.005	.003	.002	.002	.002	.002
Maximum concentration	.108	.117	.117	.093	.096	.121

Fig 3b shows the maximum and minimum predicted concentrations throughout the duration of the simulation. The largest range (50 times) in the predicted concentrations occurs after 20 hours after the spill and the predicted time to reach the safe concentration has a minimum of 7 hours and a maximum which occurred after the end of the simulation (> 40 hours).

(a) (b)

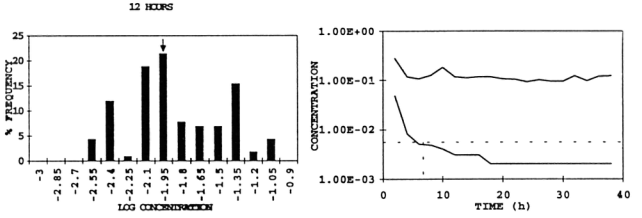


Fig 3: Predicted range of concentrations at (a) 12 hours after the spill. (b) Maximum and minimum predicted concentrations throughout the spill.

The range of predicted values for the day to day variation in mixing is larger than the range resulting from the uncertainty in the model formulation. This indicates that it would be more effective to target field investigations to determine the variability in the mixing with a number of shorter dye experiments rather than trying to carry out a few longer term dye experiments.

4 CONCLUSIONS

A random walk tidal model of the Forth estuary in Scotland has been used to investigate the uncertainty in predicted estuarine concentrations. This uncertainty is either caused by the theoretical formulation used to model the horizontal mixing or it is due to day to day variations in the mixing coefficients.

Three different formulations have been used for the modelling of horizontal mixing: in each case the model has been calibrated against data from a 6 hour dye dispersion experiment. The different methods have then been used to model the spread of a chemical in the estuary over a period of 48 hours. After approximately 6 hours the predicted concentrations

and affected area from the different formulations started to diverge, but by 48 hours the predicted concentrations had once again converged because the patch had become mixed across the whole cross section of the estuary. A maximum difference in the predicted concentrations was found to be 10 times and occurred 20 hours after the discharge. This uncertainty in the predicted concentration leads to an uncertainty in the time before a safe concentration is reached; in this example the range of predicted times for the chemical to be sufficiently diluted was from 10 to 35 hours.

A series of dye experiments in the estuary have provided information on the variability of the mixing, and data from fixed station surveys at 5 positions in the estuary over a period of 2 days on spring tides and 2 days on neap tides has given information on the variability of the tidal current. The random walk model was used to simulate the uncertainty in the predicted concentrations resulting from the variability in the measured mixing rates and tidal currents, for the same spill conditions used above. Post-processing of the model output showed the distribution of possible concentrations for a range of times from discharge. The envelope of maximum and minimum concentration values indicates a range of 50 times in the simulated concentrations and a time to safety which varies from 5 to >40 hours.

The range of predicted values for the day to day variation in mixing was larger than the range resulting from the uncertainty in the model formulation. This indicates that it would be more effective to target field investigations to determine the variability in the mixing with a number of shorter dye experiments rather than trying to carry out a few longer term dye experiments.

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TOUCHING ON A ZERO-VARIANCE SCHEME FOR SOLVING LINEAR EQUATIONS BY RANDOM WALK PROCESSES

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TRODUCTION

ference [1] the author developed a powerful algorithm for calculating derivatives in systems of linear tions describing random walk processes. The algorithm renders the first and higher-order derivatives of the iowns x_i with respect to the matrix elements p_{ij}.

In the paper presented here it is demonstrated how the derivatives constitute the essential information to mine the estimate of the inverse of the parameter matrix $\boldsymbol{R} = \boldsymbol{I} - \boldsymbol{P}$. Furthermore, it will be shown that $\boldsymbol{R}^{-1}$ be utilized (by a short iterative process) to improve both, the inverse itself and the x_i _s, so that they erge to their expectation, rendering a zero-variance result in a mainly statistical simulation procedure.

As shown in [1] a set of linear equations

$$\boldsymbol{x} = \boldsymbol{P}\boldsymbol{x} + \boldsymbol{a} \tag{1}$$

ıe solved by a Neumann series expansion obtained by the following simple algebra:

$$\boldsymbol{x}\cdot(\boldsymbol{I} - \boldsymbol{P}) = \boldsymbol{a} \Rightarrow \boldsymbol{x} = \boldsymbol{a}\cdot(\boldsymbol{I} - \boldsymbol{P})^{-1} \tag{2a}$$

$$\boldsymbol{x} = \boldsymbol{a}\,(\boldsymbol{I} + \boldsymbol{P} + \boldsymbol{P}^2 + \boldsymbol{P}^3 + \ldots) \tag{2b}$$

system of order m can be interpreted as a random walk process if the matrix $\boldsymbol{P}$ describes transition pro- lities where i and j can both assume a set of states from 1 to m.

A general method of calculating simultaneously with the $\hat{x}_i$-s the derivatives of the $\hat{x}_i$-s with respect to the s is based upon the following equation, which has like (2b) to be interpreted in terms of a random walk edure:

$$\frac{\partial \boldsymbol{x}}{\partial Q} = \frac{\partial}{\partial Q}\left(\frac{\boldsymbol{a}}{\boldsymbol{I}-Q}\right) = \boldsymbol{a}\cdot(\boldsymbol{I} + 2Q + 3Q^2 + \ldots) \quad \text{where } \frac{\partial \boldsymbol{x}}{\partial Q} \text{ stands for all } \frac{\partial x_k}{\partial q_{ij}} \tag{3}$$

ENERATION OF THE INVERSE

generation of the inverse of a large matrix is usually a lengthy and cumbersome process. Not so, however, if derivatives are known. We write $\boldsymbol{x} = \boldsymbol{P}\boldsymbol{x} + \boldsymbol{a}$ in the form an algebraic system $\boldsymbol{R}\boldsymbol{x} = \boldsymbol{a}$, where $\boldsymbol{R} = \boldsymbol{I} - \boldsymbol{P}$, $\boldsymbol{x} = \ldots, x_m)$ and $\boldsymbol{a} = (a_1, \ldots, a_m)$. Now we differentiate with respect to the elements R_{ij} of the matrix $\boldsymbol{R}$:

$$\boldsymbol{R}\delta\boldsymbol{x} + \delta\boldsymbol{R} = 0$$

$$R_{ij}\left[\frac{\partial x_j}{\partial R_{\mu\nu}}\right] = -\frac{\partial R_{ij}}{\partial R_{\mu\nu}}x_j$$

where

$$\left[\frac{\partial x_j}{\partial R_{\mu\nu}}\right] = S_j^{(\mu\nu)} = -R_{ji}^{-1}\frac{\partial R_{ik}}{\partial R_{\mu\nu}} \cdot x_k = -R_{ji}^{-1} \cdot x_k \quad \text{since} \quad \frac{\partial R_{ik}}{\partial R_{\mu\nu}} = \begin{cases} 0 & \text{for } \mu\nu \neq ik \\ 1 & \text{for } \mu\nu = ik \end{cases} \tag{4}$$

It follows that the inverse can be expressed as

$$R_{ji}^{-1} = -S_j^{(ik)} \,/\, x_k \tag{5}$$

Since the index k in the equation above can take any number between 1 and m (m: number of equations), we get m estimates of the inverse $\boldsymbol{R}^{-1}$ which are denoted by $\boldsymbol{R}_k^{-1}$ and differ only by their statistical uncertainty, but converge to the same expectation. To make use of all the accumulated information the inverse is calculated as the weighted sum of all m inverse matrices $\boldsymbol{R}_k^{-1}$. As a weighting factor the sensitivities $S_j^{(ik)}$ associated with the corresponding matrix element are chosen.

$$R_{ji}^{-1} = \left[\sum_k [R_{ji}^{-1}]_k \, S_j^{(ik)}\right] / \sum_k S_j^{(ik)} \tag{6}$$

Knowing an estimate $\bar{\boldsymbol{R}}^{-1}$ of $\boldsymbol{R}^{-1}$ it is possible to approximate the inverse itself to any desired degree of accuracy by an iteration process, making use of the condition

$$\boldsymbol{R} \cdot \boldsymbol{R}^{-1} = \boldsymbol{I}. \tag{7}$$

To improve the Monte Carlo estimate $\bar{\boldsymbol{R}}^{-1}$ we calculate

$$\boldsymbol{R} \cdot \bar{\boldsymbol{R}}^{-1} = \bar{\boldsymbol{I}} \tag{8}$$

where $[\,\bar{r}_{ij}\,]^{-1} = [\,r_{ij} + \delta r_{ij}\,]^{-1}$ and $\bar{i}_{ij} = i_{ij} + \delta i_{ij}$. Subtracting Equation (7) from (8) we get $\boldsymbol{R} \cdot \delta\boldsymbol{R}^{-1} = \delta\boldsymbol{I}$, and consequently

$$\delta\boldsymbol{R}^{-1} = \bar{\boldsymbol{R}}^{-1} \cdot \delta\boldsymbol{I} \tag{9}$$

Subtracting $\delta\boldsymbol{R}^{-1}$ from $\bar{\boldsymbol{R}}^{-1}$ renders an improved estimate of $\bar{\boldsymbol{R}}^{-1}$. The procedure can be repeated until all δr_{ij} are less then an arbitrarily small ε. Now, the exact values for the x_j -s can be obtained directly by matrix algebra.

If the exact value of the inverse matrix is not required, its estimate $\boldsymbol{R}^{-1}$ can be used to improve the $\hat{x}_j$-s directly. To this end we insert the $\hat{x}_j$ -s into our system of linear equations and calculate $\hat{a}_i$. We write $\hat{x}_j = x_j + \delta x_j$ and $\hat{a}_i = a_i + \delta a_i$, where δa_i is the deviation of the estimated $\hat{x}_j$ from the expectation x and δa_i the difference between $\sum_j r_{ij}\,\hat{x}_j$ and a_i

$$r_{i1}\,(x_1 + \delta x_1) + r_{i2}\,(x_2 + \delta x_2) + \ldots \;=\; \hat{a}_i \tag{10}$$

From this equation we subtract

$$r_{i1}\,x_1 + r_{i2}\,x_2 + \ldots \;=\; a_i \tag{11}$$

and obtain

$$r_{i1}\,\delta x_1 + r_{i2}\,\delta x_2 + \ldots \;=\; \delta a_i$$

or more generally

$$\boldsymbol{R} \cdot \delta\boldsymbol{x} = \delta\boldsymbol{a} \tag{12}$$

As the inverse of $\boldsymbol{R}$ can be calculated by Equation (2) we get an estimate of $\delta\boldsymbol{x}$ directly from

$$\delta\boldsymbol{x} = \bar{\boldsymbol{R}}^{-1} \cdot \delta\boldsymbol{a} \tag{13}$$

The elements of the inverse matrix $\bar{\boldsymbol{R}}^{-1}$ are subject to uncertainties and therefore (13) may not provide the exact values of $x_j = \hat{x}_j - \delta x_j$ directly. It is, however, possible to iterate expressions (12) and (13) such that the deviation δx_j (from the expectation x_j) remains below an arbitrarily small ε.

In this procedure the inverse matrix is obtained directly from the derivatives of the unknowns with ect to the transition probabilities. The derivatives themselves are the result of a simple counting algorithm :h can be considered to be an alternative to the much more complicated Gaussian elimination technique.

The procedure is entirely based on Monte Carlo estimators and therefore subject to statistical :rtainties. But the values of the unknowns converge after a finite number of iteration steps to the :ctation, or in other words to a zero-variance estimator, quite independently from the number of histories.

JMERICAL EXAMPLE

algorithms described above were tested in a program allowing for an arbitrary number of equations (only :d by the size of the computer memory). To illustrate the method in a transparent model a 3×3 matrix :ion was solved and compared with values obtained by classical methods.

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} .25 & .50 & .40 \\ .30 & .30 & .40 \\ .20 & .20 & .20 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} .30 \\ .30 \\ .40 \end{pmatrix}$$

of Random Walks: *1000* (on purpose only a small number of random walks was chosen !)

te Carlo solution: $x_1 = 4.1370E+00$ $x_2 = 3.7440E+00$ $x_3 = 2.5520E+00$

vatives of *x(1)* with respect to: (by Monte Carlo)

	ρ(i, 1)	ρ(i, 2)	ρ(i, 3)
I= 1	3.7700E+00	7.1780E+00	3.7320E+00
I= 2	4.9140E+00	4.4630E+00	4.1070E+00
I= 3	3.1470E+00	3.0840E+00	2.1620E+00

Derivatives of *x(2)* with respect to: (by Monte Carlo)

	ρ(i, 1)	ρ(i, 2)	ρ(i, 3)
I= 1	2.5160E+00	4.9510E+00	2.5130E+00
I= 2	5.5170E+00	4.8890E+00	4.6400E+00
I= 3	2.8860E+00	2.7760E+00	1.9960E+00

/atives of *x(3)* with respect to: (by Monte Carlo)

	ρ(i, 1)	ρ(i, 2)	ρ(i, 3)
= 1	1.5990E+00	3.1250E+00	1.6250E+00
= 2	2.7460E+00	2.5640E+00	2.2960E+00
= 3	2.5880E+00	2.5900E+00	1.7550E+00

rse of *P* (by Monte Carlo):

= 1	3.7404E+00	3.9835E+00	4.0307E+00
= 2	2.5452E+00	4.4461E+00	3.6777E+00
= 3	1.6185E+00	2.2473E+00	3.3301E+00

Inverse of *P* after *3* Iterations

I= 1	4.0000E+00	4.0000E+00	4.0000E+00
I= 2	2.6667E+00	4.3333E+00	3.5000E+00
I= 3	1.6667E+00	2.0833E+00	3.1250E+00

oved Values for Unknowns:

: *4.0000E+00* $X_2 = 3.5000E+00$ $X_3 = 2.3750E+00$

omparison: *Matlab®* renders for $x_{j=1\ to\ 3}$, R and its inverse R^{-1} the following "exact" solutions:

$$\begin{matrix} x_1 = 4.000 \\ x_2 = 3.500 \\ x_3 = 2.375 \end{matrix} \quad R = \begin{pmatrix} 0.75, & -0.50, & -0.40 \\ -0.30, & 0.70, & -0.40 \\ -0.20, & -0.20, & 0.80 \end{pmatrix} \quad R^{-1} = \begin{pmatrix} 4.000, & 4.000, & 4.000 \\ 2.667, & 4.333, & 3.500 \\ 1.667, & 2.083, & 3.125 \end{pmatrix}$$

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BAYESIAN SENSITIVITY ANALYSIS: A REVIEW

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1 SENSITIVITY ANALYSIS IN BAYESIAN ANALYSIS

We adopt the standard Bayesian decision theoretic framework, see [1]. We assume that we have to choose among a set $\mathcal{A}$ of alternatives a, according to their posterior expected utility. For that, we assess the prior beliefs on a state variable $\theta \in \Theta$ in a prior distribution π_0. They are updated to the posterior $\pi_0(\cdot|x)$, where x is the result of an experiment with likelihood $l(x|\theta)$ over a sample space X. We associate a consequence $c \in C$, to each pair (a, θ). Preferences over consequences are modelled with a utility function u_0, and we associate with each alternative a its posterior expected utility:

$$T(u_0, \pi_0, a) = \frac{\int_\Theta u_0(a,\theta) l(x|\theta) d\pi_0(\theta)}{\int_\Theta l(x|\theta) d\pi_0(\theta)}.$$

We maximize $T(u_0, \pi_0, a)$ with respect to a, as a way of obtaining the optimal alternative a^*.

However, the assessment of u_0 and π_0 is far from simple and we shall need tools to check their impact on the optimal alternative. This has been widely acknowledged in the Bayesian arena, leading to a vast literature on Bayesian robustness and sensitivity analysis, see [2], [3] and [4] for reviews. Note, though, that these studies have concentrated mainly on inference issues and, therefore, in sensitivity to the prior. In this paper, we review the field with a decision theoretical perspective and emphasis on developments since the reviews mentioned above.

2 BAYESIAN SENSITIVITY ANALYSIS: SOME MYTHS

Simple examples show that a number of special issues arise when undertaking sensitivity analysis in this field:

- It is not enough to study changes in output by trying some other couples of utilities and probabilities.
- Partial sensitivity studies are not sufficient: a problem may be insensitive to changes in utility and changes in probability, but sensitive to simultaneous changes in utility and probability.
- When performing sensitivity analysis, there are cases in which utility may change a lot, with virtually no change in the optimal action.
- Alternatively, there are cases in which the optimal alternative changes a lot, but maximum expected utility does not change practically.
- Big changes in expected utility do not necessarily correspond to big changes in consequences of interest.
- Standard global Bayesian robustness studies [5], based e.g. on ranges of expected utilities of actions, may not be sufficient within a decision theoretic perspective.

3 FOUNDATIONAL QUESTIONS

The above issues suggest we should show some care when addressing sensitivity analysis questions within a decision theoretic framework. A way forward is to reconsider the foundations of the robust Bayesian approach. These essentially suggest that beliefs may be modelled by a class of probability distributions, that preferences over consequences may be modelled by a class of utility functions and that preferences over alternatives may be modelled by the class of expected utilities, see [6].

4 CLASSES

A natural question would therefore be the study of such classes. Several authors, see e.g. [4], have dwelt on desirable properties of classes of priors. Similar issues might apply to classes of utility functions. Perhaps the basic property should be that they are related to assessment methods. As a consequence, we suggest using parametric classes for both preferences and beliefs, quantile classes for beliefs and partially assessed utility functions. The rest of the study uses various combinations of these classes.

5 COMPUTATION OF NONDOMINATED ALTERNATIVES

The main consequence of the foundational principles mentioned above are that we should look for nondominated alternatives. We suggest a scheme for approximating the nondominated set and study its implementation for our classes of interest. Relations with the set of Bayes actions will be considered.

Note that, as a byproduct of these computations, we find out whether there may be changes in the optimal alternative, and estimates of differences in expected utility.

6 EXTRACTING ADDITIONAL INFORMATION

It may happen that there are several nondominated alternatives and differences in expected utilitites are non-negligible. If such is the case, we should look for additional information that would help us to reduce the classes, and, perhaps, reduce the nondominated set. We shall describe tools based on functional derivatives, like in [7] and [8], to elicit additional information.

7 MAXIMIN SOLUTIONS

It may happen that we are not able to gather additional information, yet there are several nondominated alternatives with very different expected utilities. In these situations, maximin solutions may be useful as a way of selecting a single robust solution. We associate with each alternative its smallest expected utility; we then suggest the alternative with maximum smallest expected utility. We describe in some detail properties of maximin solutions and procedures to compute them.

8 STABILITY THEORY

Stability theory aims at formalising if an elicitation problem is nonrobust. Different notions of stability are presented in [9] and in [10], where conditions are found such that uniform convergence of losses implies convergence of optimal decisions.

9 OTHER APPROACHES

Other usual SAMO approaches, e.g. response surface methodologies, have a role in sensitivity analysis in Bayesian analysis as we shall describe.

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MULTIPARAMETRIC SENSITIVITY ANALYSIS IN THE MOIRA SYSTEM

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1 INTRODUCTION

MOIRA is a system supporting the identification of optimal remedial strategies for restoring radionuclide contaminated aquatic ecosystems and drainage areas. Possible interventions may result in detrimental ecological, social and economical effects. Decision makers (DM) must evaluate carefully these impacts. This task may be difficult, hence the need of developing a system as MOIRA which facilitates decision making.

The basic methodology is decision analytic, see [1]. Preliminary studies suggest little uncertainty in policy effects, so we consider our problem under certainty and use a multiattribute additive value function to rank strategies. Since the assessment of weights and component values is far from easy, we use sensitivity analysis methods to alleviate this task, allowing decision makers to gain insights into the problem.

The methodology has been implemented in a PC based Decision Support System (DSS) which will allow the incorporation of all relevant information in the process.

2 BASIC RANKING MODEL

A hierarchical structure with seventeen objectives has been built to evaluate countermeasures. To facilitate assessment and understanding, objectives were arranged in different levels. Hence, relevant consequences of a countermeasure S_l will be described by a vector $(x_1^l, ..., x_{17}^l)$, where x_i^l is the level of S_l in the i-th attribute.

Since an additive value function may be considered as a valid approximation in our case, see [2] and [3], we shall use the evaluation

$$v(S_l) = w_1 v_1(x_1^l) + w_2 v_2(x_2^l) + \cdots + w_{17} v_{17}(x_{17}^l) \quad (1)$$

where v_i's are component value functions and w_i's are weights or scaling constants for each component value function

The assessment of component value functions combines the probability equivalent (PE) method and the certainty equivalent (CE) method, see [4], to mitigate method dependence of the assessment, and prevent biases and inconsistencies. Moreover, rather than asking for precise preference statements, we allow for imprecision in preferences, leading to a class of value functions, instead of one. This allows simple consistency checkings and will form part of the structural bases of our sensitivity analysis. Component value functions v_i are assumed to be natural cubic splines, with parameters fitted by least squares.

Then, we assess weights for all objectives, in all levels of the hierarchy. However, as with component value functions, we allow the DM to provide intervals for the weights rather than precise values, i.e.,

for level j and objective i the DM has to provide an interval $\left[w_i^{jL}, w_i^{jU}\right]$. This is aimed at reducing the cognitive burden on the DM. The intervals are interpreted as constraints on the weights and are used later in the sensitivity analysis phase. Then, once with the specific value function we may rank countermeasures. However, since the assessment of the value function is far from simple we introduce in MOIRA sensitivity analysis tools.

3 SENSITIVITY ANALYSIS IN MOIRA

In any quantitative analysis, we may gain additional insight through sensitivity analysis (SA). MOIRA provides three types of sensitivity analysis that we shall briefly describe next.

MOIRA evaluates a strategy S_l described by $(x_1^l, ..., x_{17}^l)$ and its value in each attribute, by means of the additive value function (1). Component functions were assessed obtaining estimates for several values of X_i, say x_{i*}, x_i^I, x_i^{II}, x_i^{III}, x_i^*, (where x_{i*} and x_i^* represent, respectively, the least and most preferred consequences for attribute X_i, and x_i^I, x_i^{II}, x_i^{III} are three intermediate values) by two methods (PE and CE), obtaining a class of value functions, defined by constraints $v_i\left(x_i^j\right) \in \left[v_i^{jL}, v_i^{jU}\right]$, taking the mid-point in the interval, and then fitting a certain parametric curve

$$v_i(\cdot) = v_i(\cdot, a_i, b_i, c_i, d_i)$$

where (a_i, b_i, c_i, d_i) is a vector of parameters. Ranges on values provide implicit ranges on those parameters for $i = 1, ..., 17$, i.e.

$$v_i(x_i, a_i, b_i, c_i) \in \left[v_i^{jL}, v_i^{jU}\right], \quad j = I, II, III \tag{2}$$

which will be denoted by $\mathbf{v} \in V$. Then, weights w_i are assessed leading to ranges

$$w_i^j \in \left[w_i^{jL}, w_i^{jU}\right] \tag{3}$$

We shall denote with $\mathbf{w} \in W$ such set of constraints.

These imprecise values and weights will be used in SA to gather information and help the DM to choose a strategy. We shall describe three types of complementary SA available in the MOIRA system. Each one is more sophisticated than the former, in the sense of better exploiting the information available on the inputs.

3.1 Trying other values

The simplest way of performing SA, see e.g. [5], consist of changing the values of weights (or other relevant parameters), and observe their impact on the ranking on alternatives. Suppose the DM introduces a change in a weight w_i^j for level j objective i or in the normalized weight range $\left[w_i^{jL}, w_i^{jU}\right]$. MOIRA cares for how these changes must be propagated in the objectives hierarchy and recalculates the overall value for each strategy.

This type of SA may provide some help to DM, specially if little sensitivity to changes in weights (or other parameters) is detected. Alternatively, we may view it as an opportunistic way of finding potentially optimal alternatives (see subsection 3.3)

3.2 Visual interactive sensitivity analysis

VISA, [6], provides a SA in which the effects of changing weights and values of alternatives may be visualized interactively. VISA is a multicriteria decision support system based on a multiattribute value function. An important and distinctive feature is its extensive facility for visual interactive sensitivity analysis, which enables DMs to explore on-line implications of changing weights and values, providing an easy way to investigate sensitivity issues. VISA assumes an additive value function, with precise values and weights. It is possible to consider simultaneous changes on weights and/or values to gain insight in the problem. The whole process may be done through a graphical interface.

3.3 Full SA

The above sensitivity analysis is helpful but somehow unguided. At the same time, it provides lots of useful information that could be exploited. Essentially, through VISA type explorations we may determine some more constraints on weights and values, to be added to (2) and (3). Then, they may be used in computations described in [7] and [8], to eliminate definitely bad strategies, mainly discard dominated strategies and/or non potentially optimal.

For that, let us rewrite

$$v(S_l) = v(S_l, \mathbf{w}, \mathbf{v})$$

and if $(x_1^l, ..., x_{17}^l)$ is the consequence for strategy S_l and $(x_1^q, ..., x_{17}^q)$ is for S_q, we will check whether strategy S_q dominates S_l ($S_l \prec S_q$), by solving the optimization problem

$$[P_{lq}]: \begin{cases} \min & z_{lq} = v(S_q, \mathbf{w}, \mathbf{v}) - v(S_l, \mathbf{w}, \mathbf{v}) \\ \text{s.t.} & \\ & \mathbf{w} \in W,\ \mathbf{v} \in V \end{cases}$$

If the optimal value $z_{lq}^* > 0$, then $S_l \prec S_q$ and we discard strategy S_l.

The system can also determine potentially optimal (p.o.) strategies among the nondominated ones. To discover whether an strategy S_j is p.o., we consider the problem

$$[P_j]: \begin{cases} \min & z_j \\ \text{s.t.} & \\ & \mathbf{w} \in W,\ \mathbf{v} \in V \\ & v(S_j, \mathbf{w}, \mathbf{v}) - v(S_k, \mathbf{w}, \mathbf{v}) + z_j \geq 0, \forall k \neq j \end{cases}$$

If the optimal value $z_j^* \leq 0$, then S_j is p.o.

Next, MOIRA may compute the adjacent potentially optimal (a.p.o.) alternatives, i.e., those that may share optimality with S^*, the strategy with highest overall value under (1). To find whether S_j is a.p.o. to S^*, we solve the problem

$$[P_j^*]: \begin{cases} \min & z_{j^*} = (v(S_j, \mathbf{w}, \mathbf{v}) - v(S^*, \mathbf{w}, \mathbf{v}))^2 \\ \text{s.t.} & \\ & \mathbf{w} \in W,\ \mathbf{v} \in V \\ & v(S_i, \mathbf{w}, \mathbf{v}) - v(S^*, \mathbf{w}, \mathbf{v}) \leq 0,\ \forall i \neq j \end{cases}$$

All these computations, help to identify the remedial strategies on which the DM should focus attention.

Finally, MOIRA computes the sensitivity index $r = \rho/\delta$, which gives us a relative measure of the insensitivity of S^* to changes in $\mathbf{w}$. The value $\rho = \min_j d_j$, where d_j is obtained solving the problem

$$[Pd_j]: \begin{cases} & \min d_j = d((\mathbf{w}, \mathbf{v}), (\mathbf{a}, \mathbf{b})) \\ \text{s.t.} & \\ & \mathbf{w} \in W,\ \mathbf{v} \in V \\ & v(S_j, \mathbf{w}) - v(S^*, \mathbf{w}) = 0 \end{cases}$$

where $\mathbf{a}$ is the estimate of $\mathbf{w}$, $\mathbf{b}$ is the estimate of $\mathbf{v}$ and d is the Euclidean metric. δ is the solution of

$$\begin{array}{ll} \min & d((\mathbf{w}, \mathbf{v}), (\mathbf{a}, \mathbf{b})) \\ \text{s.t} & \\ & \mathbf{w} \in W,\ \mathbf{v} \in V \end{array}$$

4 CONCLUSIONS

MOIRA is a comprehensive DSS to identify optimal remedial strategies for restoring water systems. It is intended for use in case of accidental introduction of radioactive substances into an aquatic ecosystem and its drainage areas. Countermeasures are then evaluated with MOIRA's evaluation module, which is based on Decision Analysis methods. A class of additive multi-attribute value functions represent

the experts' preferences. MOIRA will rank the countermeasure strategies. Moreover, we introduce the possibility of multiparametric sensitivity analyses with respect to weights and values of DMs, to aid them in choosing a final strategy. For that, we apply some concepts which permit us to reduce the set of strategies of interest and assess robustness of solution and, eventually, elicit additional information from the DMs, see [7] for some ideas.

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SENSITIVITY AND UNCERTAINTY ANALYSIS USING AN INTERVAL ARITHMETIC APPROACH

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SUMMARY

Policy Analysis is the analytical activity undertaken in direct support of specific public or private sector decision makers who are faced with a decision that must be made or a problem that must be solved. To undertake this kind of analysis the so called "ten commandments" for good analysis has been developed, one of which involves being explicit about uncertainties and perform systematic Sensitivity and Uncertainty Analysis. Classical techniques used in Sensitivity and Uncertainty Analysis include: Worst-case, Probabilistic Transformation of Variables, Moments and Monte Carlo.

This paper shows the use of Interval Arithmetic as an alternative method to calculate how system outputs vary as input parameters vary. Two examples presented show that Interval Arithmetic is able to perform sensitivity and uncertainty analysis, assigning bounds to some or all the input parameters and observing the effect on the final interval outcome, that will contain all possible solutions due to the variations in input parameters, with only *one calculation.*

1 SENSITIVITY AND UNCERTAINTY ANALYSIS

For examining the effects of uncertain inputs within a model, various analytic and computational techniques exist. These include methods for computing the effect of changes in inputs on model predictions, i.e. *sensitivity analysis,* methods for calculating the uncertainty in the model outputs induced by the uncertainties in its inputs, i.e., *uncertainty propagation,* and methods for comparing the importance of the input uncertainties in terms of their relative contributions to uncertainty in the outputs, i.e., *uncertainty analysis.*

Techniques used in sensitivity and uncertainty analysis may include: deterministic, one-at-time analysis of each factor holding all others constant at nominal value; deterministic joint analysis, changing the value of more than one factor at a time; parametric analysis, moving one or a few inputs across reasonably selected ranges such as from low to high values in order to examine the shape of the response and probabilistic analysis, using probability density functions, regressions or Monte Carlo simulation [1].

A tentative condensed list of reasons why and instances where Sensitivity Analysis should be considered can be found in [2]. In most cases sensitivity analysis does not deal with the possibility that several parameters varying simultaneously can cause significant variations in the output. However holding all variables fixed except one ignores any correlation between the existing variables. Ignoring the dependence structure could result in a compromised sensitivity analysis [3].

2 INTERVAL ARITHMETIC [4-7]

Interval arithmetic originates from the recognition that frequently there is uncertainty associated with the parameters used in a computation. This form of mathematics uses interval "numbers", which are actually an ordered pair of real numbers representing the lower and upper bound of the parameter range [5]. For example, if we know that an Interest Rate is between 12 and 15 %, the corresponding interval number would be written as follows: i = [12,15] %. Interval arithmetic is built upon a basic set of axioms. If we have two interval numbers [a, b] and [c, d] with $a \leq b$ and $c \leq d$ then:

$X + Y = [a,b] + [c,d] = [a+c, b+d]$ $\qquad$ $X - Y = [a,b] + (-[c,d]) = [a-d, b-c]$

$X * Y = [\min\{ac, ad, bc, bd\}, \max\{ac, ad, bc, bd\}]$ $\qquad$ $X / Y = [a,b] / [c,d] = [a,b] * [1/d, 1/c],\ 0 \notin [c,d]$

Only some of the algebraic laws valid for real numbers remain valid for intervals. It is easy to show that interval addition and multiplication are associative as well commutative. However, the distributive law does not always hold for interval arithmetic [6]. The failure of the distributive law often causes overestimation. For example X-X≠ 0 and X/X ≠ 1.This effect is called the "dependency problem" [7] and we need to rearrange the expression to be evaluated. For example, the expression $V_{AB} = \frac{V_0 R}{(R + R_d)}$, should be evaluated as $V_{AB} = V_0 * 1 / (1+R_d/R)$.

Consider a real valued function f of real variables $x_1, x_2, ...,x_n$ and an interval function F of interval variables $X_1, X_2, ..., X_n$. The interval function F is said to be an interval extension of f, if:

$$F(x_1, x_2, ...x_n) = f(x_1, x_2, ..., x_n).$$

The range of a function f of real variables over an interval can be calculated from the interval extension F, changing x_i by X_i. Moore [3] states that:

$$f(x_1, x_2, ..., x_n) \subseteq F(X_1, X_2, ..., X_n), \quad \text{for all } x_i \in X_i \ (i = 1, \ldots, n).$$

Sensitivity analysis is performed using Interval Arithmetic by assigning bounds (interval) to some or all the input parameters and determining the output interval, that will contain all possible solutions due to the variations in input parameters [7]. These intervals include the effects of any kind of correlation between variables and can be interpreted as worst cases values and are obtained with only *one calculation.*

3 CASES STUDY

We present two examples: One related to a financial applications and the other to an engineering problem.

3.1 A Financial Application

Brealey [8] presents an example considering the introduction of a small electrically powered car for city use. Based on data shown on Table No. 1, staff members have prepared the cash-flow forecast shown in Table No. 2. The model used to evaluate the Net Present Value (NPV) is:

INCOME = Unit_Sales * Price_per_unit = US*PU US = Share_of_Market* Size_of_car_market = SM * M

VAR_COST = Unit_variable_cost * Unit_Sales = UVC * US

Pretax_Profit = PP = INCOME - VAR_COST - Fixed_Cost - Depreciation

TAX = PP * 0.50 **Net_Profit** = NP = PP - TAX

Operating_Cash_Flow = OC=Depreciation+Net_Profit

NPV = -INVESTMENT + Σ (OC / (1+ MAR)^i) i = 1,...,10

If Minimum Acceptance Rate (MAR) is set to 10% then the NPV is $ 34.3 MM.

To conduct a sensitivity analysis, the marketing and production staff gave optimistic and pessimistic estimates for the variables, as shown in Table 1. Brealey [8] solve the sensitivity analysis problem setting the variables *one at time* to their optimistic and pessimistic values. Here we will perform the analysis using interval arithmetic.

Table 3 shows the interval associated to NPV calculated with interval arithmetic, for variations of single parameters (nominal range sensitivity). These effects on the outputs due to changes in each input are sometimes known as swing weights. Last row of Table 3 shows the NPV interval when all variables are permitted to vary

simultaneously. Note that this interval is obtained, in interval arithmetic, with only *one calculation.* Values obtained with Interval Arithmetic are equal to those found by Brealey. Figure 1 shows the swings for each variable ("Tornado" graph). Interval Calculation were performed using the Range Solver software [9].

Table No. 1: Basic Data

VARIABLE	EXP	PES	OPT
Market Size 10^6	10	9	11
Market Share	0.01	0.004	0.016
Unit Price $	3750	3500	3800
UnitVarCost $	3000	3600	2750
Fixed Cost MM$	30	40	20

EXP=EXPECTED
PES=PESSIMISIC
OPT=OPTIMISTIC

Table No. 2: Preliminary cash-flow in millions of dollar for the project [8]

YEAR=>	0	1 to 10
INVESTMENT	150	
1 - Income		375
2-Var. Costs		300
3 - Fixed Costs		30
4- Depreciation		15
5 - Pretax Profit		30
6 - Tax		15
7 - Net Profit		15
8-Oper. Cash flow		30
Net Cash Flow	**150**	**30**

Assumptions: **1)** Investment is depreciated over 10 years straight line. **2**)Income is taxed at a rate of 50 percent

Table No. 3: Sensitivity Analysis using Interval Arithmetic

VARIABLE	INTERVAL	NPV INTERVAL (MM$)
Market Size (MM)	[9, 11]	[11.3, 57.3]
Market Share	[0.016, 0.04]	[-103.93, 172.5]
Unit Price ($)	[3500, 3800]	[-42.5, 49.7]
Unit Var. Cost ($)	[2750, 3600]	[-150, 111.1]
Fix. Cost (MM $)	[20, 40]	[3.6, 65]
ALL		**[-361.9,1254]**

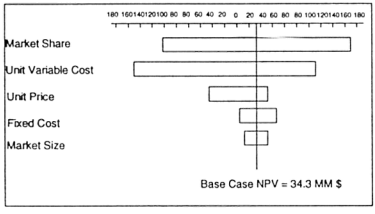

Figure No. 1: Tornado graph

3.2 An Availability Problem [10,11]

The steady-state probabilities of a continuous Markov process can be determined by solving two sets of simultaneous equations [10]: $\mathbf{A}\,\mathbf{P} = 0$ and $\Sigma P_i = 1$, where **A** is the stochastic transitional probability matrix and P the steady-state probability vector.

Figure No. 2 shows a 4-state Markov model, representing a series compensated 400 kV power line [11]. The base case reliability indices of transmission equipment used in the study are shown in Table No. 4.

We will evaluate the effect of ± 10% variations on each parameters. Bounds for state probabilities were obtained solving 2^4 = 16 times the linear systems associated with Figure No. 2 taking into account all the combinations of $(\lambda_L,\lambda_C,\mu_L,\mu_C)$.

Table No. 4: Basic Data

EQUIPMENT	λ (f/yr)	r (h/rep)
400 kV Series Capacitor	3.5	48
400 kV line	48	4

We used the interval version of the State Reduction (ISR) algorithm [9], considering λ_L, λ_C, μ_L, and μ_C as intervals with bounds calculated from base case values ± 10 %.

As shown in table No. 5, steady-state probabilities calculated with ISR are very close to those obtained by solving 16 linear systems. Also, these steady-state probabilities are included in the interval solutions.

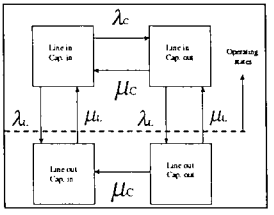

Figure No. 2: State Diagram for a Series Compensated Line

Table No. 5: Bounds for steady state probabilities

P_i	by Linear Syst.	By ISR
1	[0.9521,0.9675]	[0.951,0.9676]
2	[0.1469,0.0221]	[0.140,0.0223]
3	[0.0172,0.0257]	[0.017,0.0259]
4	[0.0024,0.0003]	[0.002,0.0005]

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BAYESIAN UNCERTAINTY ESTIMATION METHODOLOGY APPLIED TO AIR POLLUTION MODELLING

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1 INTRODUCTION

This work addresses the problem of the uncertainty of predictions of an air pollution model and their dependence on the uncertainties of observations. The uncertainty in atmospheric dispersion modelling can be related either to the uncertainty in modelled atmospheric processes and observation errors, or to the structural and numerical errors of the mathematical model. Structural errors of the mathematical model originate from the simplifications involved in the description of the atmospheric processes and differences between the scale represented by measured physical variables and the scale of their representation in the mathematical model. In the search for the physical representation of variables, scientists often forget that none of their model parameters is truly represented by the quantities measured in the field. This type of uncertainty can be accounted for, to some extent, by the application of parametric uncertainty methodology and conditioning model results on observations. However, the degree to which the uncertainties can be reduced depends on the amount of available information. Model structure limitations can substantially influence the predictions because the formulae used necessarily include simplifying assumptions which differ from reality and have been developed under specific conditions. Moreover, the random nature of atmospheric processes does not allow the model assumptions to be fully met.

The proposed methodology is based on the Bayesian Uncertainty Estimation technique (1). This method was used in hydrology as Generalised Likelihood Uncertainty Estimation (GLUE) technique, (2, 3), and it applies likelihood functions to estimate the model predictive uncertainty. The first application of the GLUE methodology to air dispersion modelling was presented in (4). The simulated model outputs are compared with the available observations of the variables of interest and the distribution of the resulting errors of predictions are used to derive the confidence limits for the predictions. The value of the confidence limits lies in their objectivity. However, as the model results depend on the information included in its input and output measurements, confidence limits will depend on the assumed input and output distributions and their ranges. Hence the choice of these distributions is very important for the reliability of the uncertainty analysis. This choice depends on the amount of available information on the modelled process. Sensitivity analysis of model variables may also be important in gaining understanding of the model performance and its internal structure. However, the sensitivity analysis on its own is not sufficient to estimate the errors of model predictions and should be followed by the uncertainty estimation techniques. The analysis of influence of different assumptions regarding model input distributions on confidence limits of the predictions can lead to the recommendations regarding the relative importance of input variables and the choice of distribution.

2 DESCRIPTION OF THE AIR DISPERSION MODEL AND DATASET

The air dispersion model described in NRPB_R91 (5), hereafter referred to as R91 is a simple and widely used Gaussian plume model applicable for short to medium range dispersion up to approximately 30 km. The model assumes that the dispersion of material is described by a Gaussian distribution characterised by standard deviations in both the horizontal and vertical directions. The standard deviations, known as diffusion parameters, are mainly dependent on the atmospheric stability. The R91 model uses Pasquill's (6) scheme for describing atmospheric stability (weather category) which gives six stability categories ranging from A, very unstable, through to F, very stable, based on measurements of wind speed, cloud cover, time of day and time of year. An estimate of the mixing layer height is assigned to each stability category and it is used by the model

when predicting the effects on ground-level concentrations caused by multiple reflections of the plume at both the surface and the top of the mixing layer. The error in the choice of the weather category is regarded as the main source of error of the predictions as it leads to different model behaviour. The determination of cross-wind spread - the standard deviation of the concentration distribution in the horizontal direction is another source of error, as the corresponding relations used in the model are derived from experiments conducted in flat terrain and the variables involved depend on the sampling times and height of measurements. In spite of these structure-dependent errors there may also be measurement errors, originating from the variability of the processes in time and space, or the necessity of introducing some data prediction where there is a lack of appropriate measurements. The other essential source of errors comes from the very limited range of data on the simulated variables, thus not allowing full calibration of the model empirical parameters.

The experimental dataset used for this study is the Copenhagen dataset selected from the Model Validation Kit used for recent model inter-comparison exercises (7). The data consist of 23 sets of ground level concentration measurements from 1 hour releases of SF_6 tracer. The experiment was performed in neutral and slightly unstable conditions. The tracer was released without buoyancy from a tower at height of 115 m. The measurements were taken for 10 distances from the source varying from 1.9 km to 6 km, in up to three cross-wind series of tracer sampling units. The value of roughness coefficient was estimated as 0.6 m. Meteorological measurements included vertical profiles of wind speed at 10 and 100 meters height.

3 THE BAYESIAN UNCERTAINTY ESTIMATION TECHNIQUE

The uncertainty analysis based on the statistical analysis of output alone (8) does not give any information about the validity of the model predictions. The uncertainty results are obtained without the use of an intermediate surrogate model by exploring the mapping from model input to model predictions. In that sense, the predictive uncertainty of the model, understood as the probable error of its predictions, is still not known. The Bayesian Uncertainty Estimation technique is the methodology which provides tools for the comparison of the model results with the observations. This methodology applies Bayes theorem to derive the predictive model uncertainties. Bayes Theorem (1) can be written as:

$$f(\theta \mid \mathbf{z}, D) = \frac{f(\theta)\, f_L(\mathbf{z}|\theta)}{f(\mathbf{z}, D)} \tag{1}$$

where z is the vector of observations, $f(\theta|z,D)$ denotes the posterior distribution of parameters θ given the observations z and input data D, $f(\theta)$ denotes the prior input distribution and $f_L(z|\theta)$ denotes the likelihood function (probability of the prediction errors understood as a function of model parameters given the observations). f(z,D) denotes the joined probability of input information and observations and can be treated as a scaling factor.

Equation (1) can be applied sequentially as new data become available and the existing posterior distribution, based on (N-1) calibration sets, is used as the prior for the new data in the Nth calibration set. This can be written in the form:

$$f(\theta|z_1,\ldots,z_N, D_1,\ldots,D_N) \propto f(\theta|z_1,\ldots,z_{N-1}\ D_1,\ldots,D_{N-1})L(\theta|z_N, D_N) \tag{2}$$

where $L(\theta/z_N,D_N)$ is the information about θ from the Nth calibration set.

Errors between the observations and simulation results together with the assumed prior distributions of parameters are used to build the posterior likelihood reflecting the model performance. In this way it is possible to incorporate the information from observations from different time periods and/or sites using the Bayesian updating described by equation (1).

In this study it is assumed that the errors between observed and predicted variables (maximum concentrations at given distances) have the additive form:

$$\mathbf{Z}_t = \mathbf{Y}_t(\mathbf{D}_t, \theta) + \delta_t \qquad t=1,\ldots,T \tag{3}$$

where δ_t is the vector of model errors. Here, δ_t is modelled by the Gaussian first order auto-regressive model AR(1) with non-zero mean μ, and auto-regressive matrix A: $\delta_t - \mu = A^*(\delta_{t-1} - \mu) + \varepsilon_t$. ε_t is assumed to be normal $N(0,\Sigma)$, with a covariance matrix Σ, T denotes a number of measurement distances from the source (4). From the error model it is seen that the likelihood function of the predicted concentrations can be expressed as the likelihood of the error variate ε with parameters $\phi = (\mu,\Sigma,A)$, depending on the air dispersion model parameters θ. Under these assumptions the likelihood function is defined as:

$$f(\theta,\phi \mid z, D) = C \times f(\theta,\phi) \times f(D) \times (2\pi\sigma^2)^{-T/2}(1-\alpha^2)^{1/2} \exp[-\frac{1}{2\sigma^2}((1-\alpha^2)(\delta_1-\mu)^2 + \\ + \sum_{t=2}^{T}(\delta_t - \mu - \alpha(\delta_{t-1}-\mu)^2)] \tag{4}$$

where C is the normalising constant, α denotes auto-regressive coefficient and $f(\theta,\phi)$ denotes the prior distribution of the atmospheric and noise model parameters.

The cumulative distribution of the error term at any time, given a particular set of atmospheric and statistical model parameters θ and ϕ, is then given by:

$$P(\delta_t < \delta \mid \theta,\phi) = \Phi\left(\frac{\delta-\mu}{\sigma/(1-\alpha^2)^{1/2}}\right) \qquad t=1,\ldots,T \tag{5}$$

where Φ is a standard normal distribution function N(0,1).
The resulting predictive distribution of tracer concentrations Z_t conditioned on the calibration data z in the discrete (parameter set) case will be then given by

$$P(Z_t < y \mid z, D) = \sum_{\theta}\sum_{\phi}\Phi\left(\frac{y-\mu-y_t}{\sigma/(1-\alpha^2)^{1/2}}\right) f(\theta,\phi \mid z, D) \tag{6}$$

From the relation (6) one can evaluate the confidence limits for the concentrations at the observation sites.

4 NUMERICAL RESULTS AND CONCLUSIONS

In the case when the range of variability is the only certain information about a variable, a uniform distribution within given ranges should be assumed. However, the parameter ranges are not certain either. The uncertainty of predictions can be decreased by conditioning of the input distributions on observations and/or conditioning of the uncertainty predictions on the output observations. The degree to which the predictions can be improved will depend on the sensitivity of model predictions to given variables. Sensitivity analysis was performed using local (one by one) and global (Monte Carlo based) methods. The results indicate that both approaches should be used simultaneously and additionally they should be combined with an analysis of the model structure. The sensitivity analysis eliminated one parameter (inversion height) from the chosen parameter set, as not influencing model predictions for the conditions corresponding to the Copenhagen dataset (i.e. within 6km of a 115 m stack in slightly unstable and neutral conditions). The uncertainty estimation was performed using marginal (summed over the noise) posterior distributions (equation 6). The variables analysed were roughness length, wind speed, release height and stability condition. In the first experiment all the variables were varied uniformly in wide ranges. The determined confidence limits for the predictions are shown on Figure 1 (x). Further on, different assumptions regarding parameter distributions were tested. The results of the analysis indicated that roughness length should be treated as a model parameter and its distribution should follow a uniform distribution on a physically feasible range. Conditioning the predictions on the release height observations significantly improves model predictions by decreasing the confidence limits. The same is true of wind speed measurements, which are the most important model variable. The analysis of the influence of wind speed distribution spread indicated that the confidence limits decrease with decrease of spread to a certain extent. This is connected with the fact that model predictions will depart from the observations if the spread of wind variations is too narrow. The confidence limits for the predictions obtained with conditioning on release height (normal priors) and wind speed observations (log-normal priors) are given on Figure 2 marked with (o).

When decreasing the confidence limits we decrease model flexibility, which is equivalent to calibration of the model results to given event data. This is not advised, as the model should give reliable predictions for a wide range of atmospheric conditions. Hence the validation of model predictions, here in the form of the confidence limits, is as important as in the case of deterministic predictions. An introduction of uncertainty in the choice of weather category gave the confidence limits (Figure 2 '+') which were the most central in respect to the concentration observations. This procedure required modification of the model structure and more detailed studies are needed to recommend the best way of representing this type of uncertainty. The introduction of observation errors which was equivalent to using the joined posteriors (equation 6) resulted in wider confidence limits for the predictions (Figure 2 '-'). The posterior probability distributions for the predictions can be used to estimate the confidence limits for the ground level concentration predictions following pollutant releases in conditions similar to the Copenhagen dataset. The results of this analysis can also provide an insight on the possible implications of the differences in atmospheric and geographical conditions on the prediction errors.

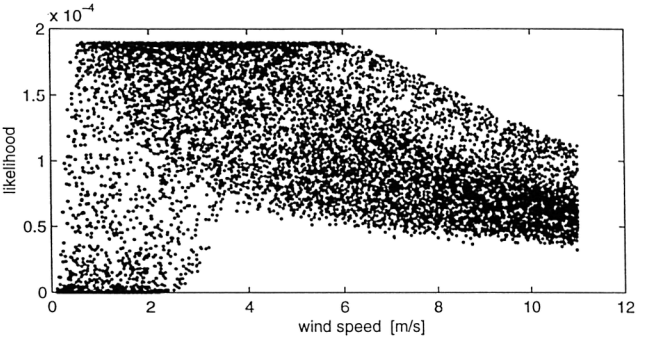

Figure 1. 95% confidence limits for the predictions for uniform distribution of parameters (no conditioning on the input observations).

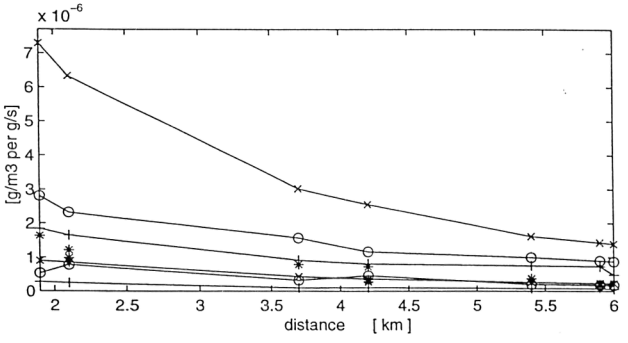

Figure 2. 95% confidence limits for the predictions: A. confidence limits conditioned on the release height and wind observations (o); B. uncertain weather category specification (+); C. included output observation errors (-); (*) denote the observations.

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ARE VARIANCE-BASED SENSITIVITY ANALYSIS METHODS HEALTHY FOR YOUR MODELS?

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1 INTRODUCTION

A combination of causes has hindered so far the effective use of sensitivity analysis for the appreciation of the sources of uncertainty affecting the prediction of a model. One is an epistemological one, another is of cultural dominance, and the third one can be termed as of practical nature.
The epistemological reason is that many different things are meant by sensitivity analysis in different user communities. For an engineer, SA could be the process of moving or changing components in the design of a plant to investigate how a fault tree analysis for that plant would change. For an economist, it is most likely the derivative of the output function with respect to the input factors. For a software engineer, SA will be related to the robustness and reliability of the software with respect to different assumptions. There is no doubt that it will be extremely hard to convince those potential users of the benefit of new SA tools unless this epistemological barrier is overcome.
The reason of cultural dominance (hegemony) is due to the predominance in the literature of the term SA used in conjunction with the concept of local derivative of output versus the input. So much so that the only review article on the subject ever published on SCIENCE (in 1989, [1]) only discussed this approach to SA. Whenever the model is nonlinear and/or the variation in the input factors non negligible, something else would be needed. Most user communities would hence argue that they do not terribly need SA, or that they have done it already with unexciting results.
The third reason, the only one I would term practical or objective, is the absence of a tool capable of global quantitative analysis. An ideal tool should in fact

- apportion quantitatively the outcome uncertainty to the input factors
- allow the factors to be uncertain over non negligible regions
- be effective independently of the model
- be computationally affordable

Such methods are now available. In this note I shall mostly concentrate on the implication of the existence of these methods, rather than describing them. Its conclusion is that those methods are very useful.

2 SENSITIVITY ANALYSIS AND EPISTEMOLOGY

In the review paper quote above, Rabitz [1] presented Sensitivity Analysis (SA) as a fundamental ingredient for model building. According to Rabitz, SA is a key tool in the understanding of a complex physical process. SA helps analysing the content of the model, and interfacing it with observational data. It also helps in identifying which dependent variable and parameter is critically important, how variables are interrelated and especially how variables at a given level of description of the system (eg quantum mechanic potentials) influence the behaviour at another -- possibly higher -- level (eg macroscopic rate constants). Rabitz also pointed out another important use of SA: the antithetical process of reducing full detailed models to their essential or lumped structures.

While Rabitz refers to SA as a 'tool' for the modelling process (either in the building or application phases), Oreskes et al., in her article on SCIENCE entitled «Verification, Validation and Confirmation of numerical models in the earth sciences» (1994, [2]), attributes to SA a different meaning. SA is not treated as a tool to build or improve a model, but it represents one of the possible licit uses that can be done of the model itself. According to Oreskes, in fact, natural systems are never closed, and models put forward as description of these are never unique. Hence, models can never be 'verified' or 'validated', but only 'confirmed' or 'corroborated' by the demonstration of agreement (non contradiction) between observation and prediction. Since confirmation is inherently partial, models are qualified by a heuristic value: models are representations, useful for guiding further study, but not susceptible to proof. Under Oreskes et al.'s point of view,

<< Models can corroborate a hypothesis [...]. Models can elucidate discrepancies with other models. Models can be used for sensitivity analysis – for exploring «what if» questions – thereby illuminating which aspect of the system are most in need of further study, and where more empirical data are most needed.>>

Rabitz and Oreskes offer us complementary definitions of sensitivity analysis: tool for the analysis for the former, substance and object of the analysis for the latter. I would like to offer a view of this discipline encompassing both aspects. My viewpoint is that the inadequacy of existing techniques (including those presented in [1]), coupled with an overconfident attitude on the side of the model developers has so far played against the use of SA. By reviewing new methodological developments in the field of global quantitative sensitivity analysis, I argue that time is ripe for a wider use of SA. My plan is hence:

1• To suggest a new paradigm for the use of model in experiments, whereby the rules of the game involving a model and the world to which it is applied are explored by the quantitative SA techniques before the experiment is enacted. This in turn will stress the importance of the use of proper quantitative SA methods as part of the model qualification process (model pedigree).
2• To offer a general but rigorous definition of what SA is, summarising disparate meanings of SA in the modelling process. I also aim to explore the tasks where SA can be useful, thus providing a sort of reference for the modeller facing one or another of the several problems solvable by SA.

Both points I and II, more in general, touch upon the merit of modelling activities in the scientific method.

3 WHAT ONE WOULD DESIRE AND WHAT IS AVAILABLE

By comparing the various methods for SA, I would argue that the following can be offered as a definition for sensitivity analysis

> **Definition:** *Sensitivity analysis studies the variation in model output variables driven by all what can be conceivably varied the model.*

A defence of this definition shall be offered in my presentation. I would also like to propose a list of «desiderata», ie of what I would regard as desirable properties in a sensitivity analysis method. The first three are offered without further preamble:

1st property, influence of scale and shape. The influence of the input should incorporate the effect of the range of input variation and the form of its probability density function (pdf). It matters whether the pdf of y_i is uniform or normal, and what are the distribution parameters.

2nd property, averaging. In the perturbative approach one computes partial derivatives: the effect of the variation of y_i when all other $y_j, j \neq i$ are kept constant at the central (nominal) value. A global method should instead evaluate the effect of y_i while all other $y_j, j \neq i$ are varying as well.

3rd property, a complete and quantitative measure. A desirable property of a global sensitivity measure would be the capacity to appreciate the so-called interaction effect, especially important for non linear, non additive models. These arise when the effect of changing y_i and y_j is different from the sum of the individual effects. In turn, appreciating the interactions is essential to the completeness of the method: the sensitivity measures for the various inputs should add up to one. The measure should hence be quantitative.

A widely used class of sensitivity tests is based on linear correlation or regression. For instance, the standard regression coefficients (SRC's) are a global measure in the sense that they take into consideration the input pdf's, and average the effect of a given factor over the variation of the others; they tend to perform poorly for non linear, non additive models. As a result another important property would be:

4th property. Model independence. The method should work regardless of the additivity or linearity of the test model.

Further analysis of the issue would suggest a further desired property:

5th property: efficiency. The measure should be computable for models of practical interest.

While shear ambition would suggest a:

6th property: agility. The measure should allow sets or subgroups of inputs to be treated as a single entity (factor).

As described at length elsewhere, sensitivity analysis possessing all the desired properties exist and are based either on Sobol' indices [3] or on an extension of FAST introduced recently [4]. These methods allow a very intuitive display of how the uncertainty in a given prediction can be broken down into constituent elements in a quantitative fashion (see Figure). Based on the existence of such a set of techniques, I would hence summarise the possible uses of SA as follws:

- To ascertain if a subset of input parameters may account for (most of) the output variance (thus allowing unimportant variables to be fixed; this was indeed the original motivation of Sobol' work [3]).
- In the same direction, global SA can used for mechanism reduction (dropping or fixing non relevant parts of the model) and for model lumping (building/extracting a model from a more complex one). This has some epistemic implications, as touches upon the «relevance» of a model. It has been argued that often the complexity of models largely exceeds the requirements for which they are used. Especially if one adopts Oreskes' viewpoint (models are heuristic constructs, built for a task), then they should not be more complex than they need to be. A model is then «relevant» when its input factors actually cause variation in the model response which is the object of the analysis. Model «un-relevance» could flag a bad model, a model used out of context, or a model unable to provide the answer being sought.
- For model identification, model selection and/or calibration. In this case SA could be also useful against ill conditioned problems.
- SA can also be used to optimally allocate resources in R&D, by showing where it is more worthwhile to invest in order to reduce the model's range of uncertainty; this is especially useful in the analysis of risk.
- Provide a quantitative hint of what fraction of prediction uncertainty is due to parametric (or aleatory) uncertainty and how much to structural (or epistemic) uncertainty.

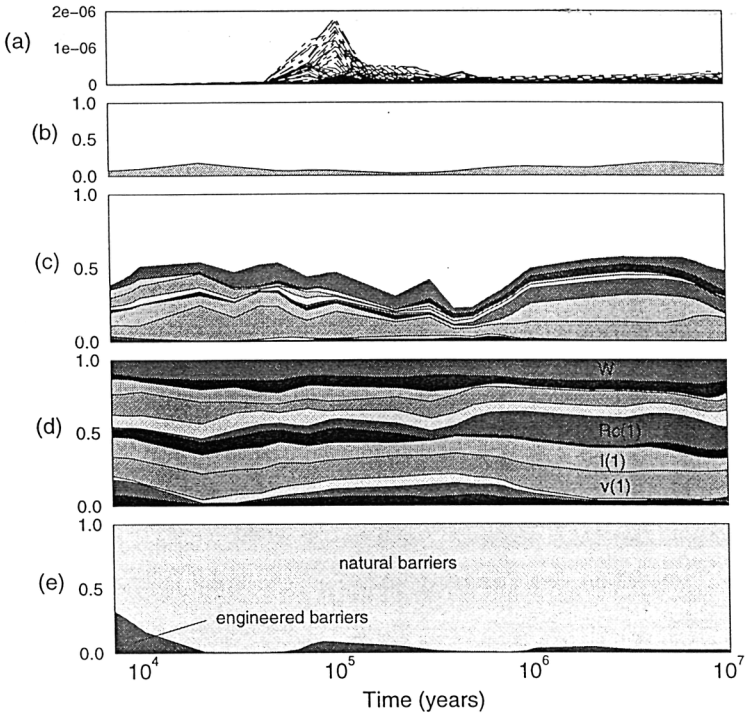

FIGURE CAPTION. The output variable considered and the model used are not relevant here. It suffices to say that the model is nonlinear. The ensemble of the frames should give a good picture of how the model behaves. (a) Are all output (y is time dependent) as function of time for several simulations. Frame (b) gives the model coefficient of determination referred to the regression model based on all the 12 factors. (c) and (d) give the cumulative representation of first order and total normalised indices, respectively (sample size 257). The sum of the first order indices (coloured region in (c)), is below 0.5 everywhere, ie the model is not additive. (e) is the cumulative representation of the total normalised indices where the factors are grouped in two sub-sets (natural and engineered barriers) in the example.

4 CONCLUSIONS

Uncertainty is not an accident of the scientific method, but its substance. Models as heuristic tools designed for a scientific task must be proven capable to deal with it. Especially when the model is used to drive a choice or a decision, the importance of the associated uncertainties should be quantified, and the relevance of the model ensured. Quantitative global sensitivity analysis could be of use in this context. I have the impression that the scientific community overestimates the merit of calibration in the context of the scientific use of models. Very often the use of model is forced within an optimisation context, where the issue is to find some least square solution to estimate the input factor which disagree less with observation. Any model must include false and or unrealistic assumptions in order to be of practical use (ie in order to «close») and these will not be made explicit in the calibration process.
Before the total sensitivity indices were introduced, there was perhaps some pretext not to run a full SA. The pretext is now fallen, and it should not be accepted that model complexity and model corroboration be presented as conflicting: the more complex a model, the less likely its corroboration. Increasing computer capacity on one hand, and epistemic awareness on the other, demand that model's relevance become a prescription for the correct use of models.

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ENVIRONMENTAL MODELS AND THEIR UNCERTAINTIES: SOURCES AND QUANTIFICATION. THEIR ROLE IN ENVIRONMENTAL IMPACT ASSESSMENT

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1 INTRODUCTION

Environmental models provide tools which synthesise data, allow predictions of behaviour, and give input to decision-making processes in environmental management. As such, they are simplifications of a complex reality and are imprecise, with many sources of uncertainty including measurement imprecision, structural and parametric uncertainties. Nevertheless, a verified, calibrated model can make a substantial contribution to environmental management. There are a large number of reasons for modelling the environment including: description of a possibly complex environmental system and the interactions between components and testing hypotheses concerning its behaviour and response to anthropogenic induced change. Under this latter reason, is included impact assessment where models have a particularly important role. In the process of environmental impact assessment (EIA), models provide one of the few tools which can be used to predict impact, and indeed to detect impact after the initiating event has occurred. In this brief note, the role of models and assessment of their uncertainties is discussed in the context of EIA.

2 ENVIRONMENTAL IMPACT ASSESSMENT (EIA)

The process of EIA can be broken down into a number of stages:

- Project design and planning;
- Baseline environmental survey;
- Impact prediction: modelling;
- Decision making process.

These may then be followed by an impact audit.

The main modelling input comes in the prediction of impact, after the targets have been identified. It has two objectives: prediction of the magnitude of impact and its importance. Its aim is to provide a clear and precise measure of impact and to attach uncertainty to the estimate. The decision concerning the importance or significance of the impact is not a statistical or modelling one, but it will be based on the modelling work done, as well as consideration of other factors (political, social and economic).

There are a wide variety of predictive methods and approaches which may be adopted in the prediction of impact. The choice of method is determined by available information, knowledge and applicability to the particular context in which the project is set. All will involve combining available environmental information of different provenance, and this also introduces further challenges in that the information may have been collected under very different protocols and may have widely varying properties. A structure under which they may be combined is required [1].

The different sources of information include:

a) expert judgement. Information based on prior knowledge, expert judgement and the environmental context within which the problem is posed all must be combined. The elicitation of expert judgement can prove difficult, and there is considerable interest in and literature about the elicitation of prior information [2].
b) comparison with other similar developments. Similar sites and developments may be assessed to provide information which may be applicable to the specific project. Difficulties arise here since it may be difficult to find comparable sites, or to decide whether two sites are directly comparable.
c) on-site experiments. As part of the EIA, site specific experiments may be carried out, tracers may be introduced and monitored to better characterise the behaviour of the system.
d) mathematical models. Change may be predicted using mathematical models. They may be complex, physically based models (e.g. climate change models) or they may be relatively simple empirical models.

2.1 Environmental modelling

Within the EIA framework, the modelling process may be iterative, with four main stages: design, conceptualisation, estimation and verification. Each stage may depend on the different information sources; expert judgement may be used to design and conceptualise the model, on-site (or site-specific) experiments can often provide information useful in parameter estimation and model verification. At each stage, however, decisions concerning structure and input must be made and at each stage uncertainties will be introduced.

2.2 Design of a Conceptual Model

The model must be fit for the purpose for which it will be used, and so we must clearly define our objectives: 'Why model the environment?' Answers could include:

- to predict the transfer of pollutants through the environmental system;
- to study the dynamics of the system;
- to synthesise different (and perhaps) conflicting data sets;
- to provide a decision-making tool.

2.3 Conceptualisation

This stage includes visualisation of the structure, identification of the processes and parameters which will be included. Following the definition of the conceptual model comes the computational representation and numerical solution, however the model will almost certainly contain unknown quantities which must somehow be estimated.

2.4 Parameter Estimation

The sources of information for parameter estimation can be many. In some situations there will be sufficient experimental data available to estimate all the parameters, however it should be borne in mind that later new data will be required for model testing. More typically, only limited data will be available, which may in itself require to be interpolated to allow parameter estimation. Such information can be supplemented by expert opinion, review of the literature or comparison with analogues. This stage is sometimes described as the calibration stage.

2.5 Validation

This is one of the most important stages in the modelling process. The modeller must demonstrate that the model is appropriate for the purpose by showing that the model will reproduce to an acceptable standard, the real world as observed. The validity may be checked using goodness of fit techniques, but should also include evaluation of the appropriateness of any assumptions made.

3 HOW GOOD IS THE MODEL?

This question is a difficult one to answer, since there are many aspects of goodness, one of particular interest is the reliability of the model. The reliability of the model can be defined by three questions:

- How large is the uncertainty associated with the model predictions?
- Is the uncertainty acceptable for decision making?
- What are the main factors contributing to the uncertainties?

Factors affecting model reliability include how the problem was specified, the formulation of the conceptual model (were important processes omitted, was a process inadequately described, are the model assumptions satisfied, is the model credible), formulation of the computational model (errors in software and codes, do the model predictions seem reasonable) and estimation of parameter values (do the predictions seem reasonable) and finally how uncertain are the results. This is perhaps the most important of the model evaluation phases, since the modeller must communicate confidence and understanding to the decision maker.

4 MANAGEMENT OF UNCERTAINTY

As we have seen, uncertainty is introduced at every stage of the evaluation process and plays a part in every decision which is to be made [3]. We can broadly categorise the sources of uncertainty.

4.1 Sources of Uncertainty

Uncertainty can enter at stages of the modelling process.

a) how to describe an effect. This is of particular importance since decisions are made about the information required and degree of precision required.

i) data collection is vital and may introduce uncertainty. There may be inherent variability in the attribute of interest, and in the measurement or collection process, uncertainties can be introduced.

) predictive methods involve a model of some type, these models cannot reproduce exactly what happens. Different types of uncertainty may be introduced in the modelling work: omission of certain processes, hence over-simplification; mathematical description of the process may be subject to uncertainty; resolution uncertainty (i.e. the model may have one level of space or time resolution while the data collected may be at another). Some of these uncertainties are irreducible, but the overall uncertainty should be evaluated.

.2 Quantification and assessment of uncertainty

he key tools in quantification and assessment of uncertainty are those of sensitivity and uncertainty analysis (SA nd UA). A number of techniques have been developed which are widely applicable which allow the empirical imulation of uncertainty (typically represented by a probability distribution of outcomes) and the evaluation of the elative contributions to the overall uncertainty made by the different parametric sources [4, 5]. There have also een a number of developments in evaluation of the contribution to the overall uncertainty due to the model tructure, both from a general Bayesian framework [6] and from empirical studies [7, 8]. Thus the tools of SA and IA provide essential information in the modelling process.

WHAT ROLE DOES UNCERTAINTY PLAY IN EIA?

he uncertainty of the model prediction has an important role to play in EIA, which cannot be ignored. There are number of sources of uncertainty, including uncertainty on data and uncertainty on models (are assumptions ppropriate, are the model variables correctly identified, is anything missing, how are the different input variables elated, what data is available?). EIA needs 'usage of prediction techniques, which yield a range of predictions nd associated probabilities for those predictions to occur' (9). Uncertainty in prediction disappears when the roject is implemented. However, it reappears when we consider the detection of impact, since there is uncertainty n sampling and observations and in the demonstration of causality.

he key environmental management question is whether the uncertainty can be managed within defined acceptable mits?

.1 Environmental Management questions or the inference problem

t is important to consider the types of management questions and how they are formulated and indeed how the odel predictions and their uncertainties can be used to answer such questions.

n a general setting, the objectives of any environmental study which involves modelling can be broadly classified s:

description and characterisation of the state of the environment; this may require a simple underlying model, such as the distribution of the characteristic of interest, or more complex spatial models for interpolation and mapping; the uncertainty may result from the natural variability in the environment, or e.g. the coarseness of the spatial information where the latter can be managed and reduced, while the former cannot.

prediction of the condition or state of the environment as a result of an activity (which may include doing nothing); the model provides a predictive tool. The certainty (or uncertainty) concerning the final condition (in terms of global concentration level) can be described in the form of a prediction interval with a specified level of confidence. Such an interval can be used to compare different predictions obtained under the different management options. The model may also be used in the process of deciding which action to undertake (e.g. in an accident situation where there is only limited data available in the early stages, a model can be used to predict likely concentrations and whether they will exceed action levels).

detection of change (within both a space and time framework); the uncertainties concern the type and magnitude of change, and our ability to measure such a change given the various uncertainties. Formal tests may be used as decision tools, and the decision will be subject to type I and type II errors. Before carrying out such a test, we must define the magnitude of an environmentally meaningful change, the precision (or uncertainty or variation) on the attribute, as well as an acceptable level for a type I error.

study of effect; in this context we may be dealing with a regulatory situation, where standards are set to protect the environment. Much of the focus for setting standards is model based. The magnitude of impact which is deemed environmentally significant is identified. It is then necessary to work back though a chain of receptors to identify the limit of release which can be set. This may require a linked series of models, where output from one model may be used as input for the next. The uncertainties at each stage must be propagated. From another perspective, having set the standard, then it is also important to identify the means of testing for compliance.

The uncertainties in a) the standard and b) its effect and c) the testing procedure all must be considered in the compliance procedure. A recent recommendation was that the standard and its testing procedure should be phrased in a probabilistic way, taking account then of the underlying uncertainties and to ensuring that the type I and type II errors are acceptable [10].

6 CONCLUSIONS

Within the context of environmental management, models play a fundamental role. The type of model ranges from a simple conceptual model (involving ideas of population and sampling unit and variation) to much more complex conceptual models of environmental systems. Nonetheless, regardless of the type of model, uncertainty is ubiquitous. At the most basic level, uncertainty is introduced when considering whether the model is appropriate for the stated objective (i.e. will meet that objective within acceptable boundaries), or whether other models might be equally acceptable competitors. At the next level, there is uncertainty concerning the parameters used within any given model, and finally at the measurement level, there is uncertainty (or perhaps more appropriately expressed, variation) in the data itself, some of which is due to the measurement procedure. Management of uncertainty must operate at all levels, not just simply the parameter level (where methods have until recently been best developed).

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SENSITIVITY ANALYSIS OF PEFORMANCE PREDICTIONS IN DISTRIBUTED APPLICATION MODELS

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ABSTRACT

Large distributed computer systems are important to industry and society. The design of these systems is a severe challenge and sensitivities can play a big role in creating robust designs. System parameters such as the computational work for a user request may be difficult to determine, or may change as users become more sophisticated, therefore having a severe impact on system performance. In addition, the behaviour of these applications can depend on hundreds of different system parameters. For a designer the impact of design parameters on performance predictions can be non-intuitive and challenging. This work uses a Layered Queueing Network model of any distributed application, and determines (and ranks) the sensitivities of a large set of performance measures such as response times and throughputs, to a large set of workload parameters for the software. As a result, designers can be provided with solid feedback, and software performance engineering can begin as early as possible in the system development cycle.

In summary, sensitivity analysis can be useful for the following:

- Determine the most sensitive parameters in the system
- Identify areas where changes can be made to improve system performance and identify hot spots
- Use sensitivity information for system optimization (ie. gradient based optimization)
- Identify areas of risk to guide future design and development

1 BACKGROUND

The performance of distributed systems is heavily influenced by message queueing and blocking. A special model called Layered Queueing Networks (LQN) which combines both queueing and blocking effects for modelling distributed applications was developed. LQN modelling provides a transparent representation of the software architecture, which makes models easy to develop and understand and represents *logical resources* such as processes, critical sections or locks. A number of tools (e.g. LQNS (1), MOL (2)) exist that support the LQN framework, however none have support for performing a sensitivity analysis. This research integrates a sensitivity analysis approach into the existing Layered Queueing Network (LQN) modelling framework.

The components of a LQN model will be described using a client-server example given in Figure 1(a). Parallelograms represent operating system processes. Processes are assigned to processors and are divided into three groups: *pure clients* (Client), *active servers* (S1) and *pure servers* (P1). Pure clients, also called reference tasks, only send requests. These tasks cycle continuously performing computation work, sleep or send requests as shown in Figure 1(c). The intent of a pure client is to model actual users or types of input sources of a system like cpu's or disk's. *Pure servers* only receive requests and they represent devices or stations found in conventional queueing networks. Finally, active servers can be thought of as a combination of clients and servers. Active servers are software processes that can both receive and generate requests.

The structure of a LQN model can be decomposed into several coupled Queueing Network submodels as shown in Figure 1(b). Parameters of a submodel are computed from results of other submodels in an iterative scheme. The method adopted here first analyzes the sensitivities of each submodel, and of the couplings between the submodels, and then combines the partial results.

Sensitivity analysis for Queueing Networks (QNs) has been reported by several authors but only for *product-form* or *separable models*, which can not directly represent systems with logical resources. QNs have been used in the modelling and analysis of these types of systems. Lui and Nain in (3), studied the sensitivity of

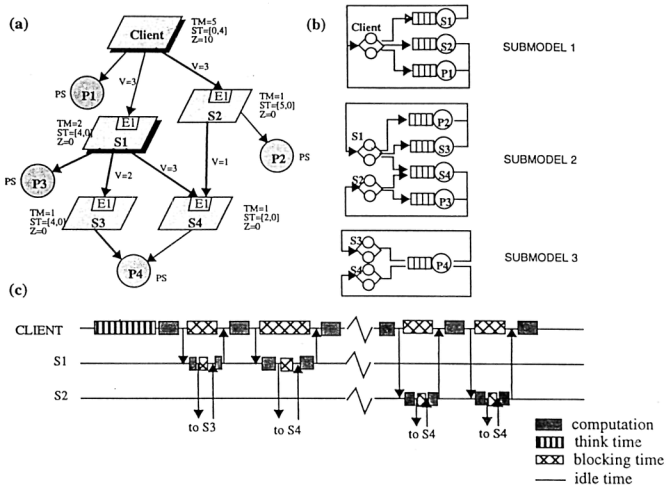


Figure 1 **(a) Layered Queueing Model (b) Decomposed Queueing Network Models (c) Execution Sequence Diagram**

performance measures of the network with respect to input parameters such as arrival rates, service times, population etc. for product form queueing networks. A number of studies where partial derivatives of queueing measures in product-form queueing networks have been carried out. Trivedi et al in (4) considered optimal selection of CPU speed and device capacities so as to maximize throughput. In (5) the aim was to maximize system throughput by routing and load balancing.

Andreas Opdahl, in (6), presents an approach to software performance modelling based on annotating the design specifications with performance parameters and operational analysis of queueing networks representing the hardware. The approach to sensitivity analysis that is presented in the paper is used to point out where model refinement and parameter capture effort should be focused and suggests performance optimizations in the design specifications. Sensitivities are obtained by differentiation of the combined software and hardware performance model, but open queueing networks are only considered at the hardware level. This approach also does not consider queueing for logical resources such as processes, critical sections, locks etc. By annotating the software design with the performance parameters, the workload on the underlying hardware can be determined but the notion that queueing can occur at software resources is not captured.

Opdahl points out that contemporary approaches to software performance engineering have weak penetration into the software development cycle. The approaches are time and knowledge intensive because they suffer from the following problems:

- the effort required to establish a software performance model
- the cost of capturing parameters for a model
- difficulty in exploiting the model to actually improve the design

Sensitivity analysis addresses the latter two points by indicating where model refinement and parameter capture effort should be focussed, and it also suggests performance optimizations in the design specification.

2 SENSITIVITY IN LAYERED QUEUEING MODELS

The example system in Figure 1(a) is used to demonstrate the approach. Sensitivity will be determined for variations in model parameters such as:

- average cpu demand of processes (ST)
- average number of requests from one process to another (V)
- population of processes (users, clones, or threading levels) (TM)
- client think time (client time between successive requests) (Z)

The performance metrics or outputs of a model are:

- response times to a service request at any level
- throughput of a process
- utilization of any hardware or software resource (cpu, task, thread)
- queue lengths at any resource

The solver uses multiple submodels, K, and an iterative solution technique. Each submodel is represented by a set of M equations. These equations are solved to arrive at the submodel solution. The outputs of submodel i, denoted by the vector $y^{(i)}$, are a function of inputs $x^{(i)}$ of that submodel, its outputs, and the outputs of other submodels, $u^{(i)}$.

$$y^{(i)} = f^{(i)}(x^{(i)}, y^{(i)}, u^{(i)})$$

$u^{(i)}$ is defined to be a function of outputs of all other submodels except submodel i.

$$u^{(i)} = g(y^{(1)}, \ldots, y^{(K)})$$

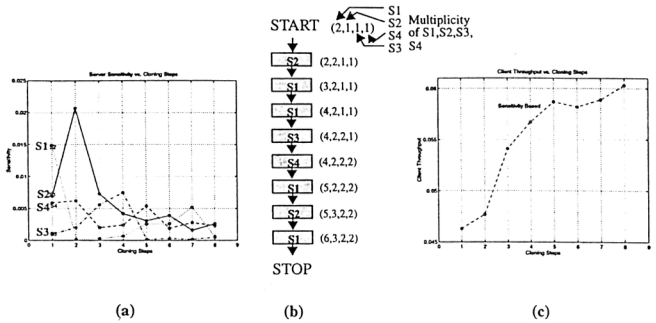
To determine sensitivities the solver was modified to output partial derivatives, $\partial y^{(i)}/\partial x^{(j)}$, of the queueing equations which define the function $f(i)$ used in each submodel along with the partial derivatives are combined with the partial derivatives of the equations from other submodels $\partial u^{(i)}/\partial y^{(j)}$. This information was then assembled to form a so-called System Matrix. This was then simplified using sparse matrix techniques to give sensitivities of all outputs of any submodel to an input of any submodel. The sensitivities can then be ranked or even be used as inputs to determine parameter elasticities, or in optimization.

A ranking of sensitivities or elasticities can then be used to identify most sensitive parameters in the system, identify bottlenecks in the system, and it can also tells us how much a particular output parameter will change to a change in an input parameter.

3 EXPLOITING THE SENSITIVITY INFORMATION

The throughput of a system can typically be improved by introducing more replicas or threads or clones of software processes. The vector $(M_1, M_2, \ldots, M_n)$ defines the multiplicity of all the servers in the model where n is the number of servers in the model. Therefore, if every server in this example had a multiplicity of two then the clone set of the system would read as (2,2,2,2). Sensitivity information was used in Figure 1(a) to determine which software server to clone. The goal was to optimize Client throughput. A sequence of eight changes were made such that at each stage a particular software server was cloned. At each stage the most sensitive multiplicity was increased by one. The layered model was then re-solved with the new clone set.

In Figure 2(a) the sensitivity of Client throughput with respect to the various M_i is given. As the number of cloning steps increase, the sensitivity of the servers can either go up or down. In this particular case server S2 was the most sensitivity to start off with. Once its multiplicity was increased, the sensitivity of server S2 decreased and the sensitivity of S1 increased. Server S1 was then selected as the next candidate to clone. In general, Client throughput becomes less sensitive as the number of server clones are increased. This indicates the movement of a potential bottleneck from one resource to another.



(a) (b) (c)

Figure 2 (a) Server sensitivity at each cloning step (b) Cloning steps with Server multiplicity (c) Client throughput at each cloning step

Changes in Client throughput at each of the eight stages can be found in Figure 2(c). The sensitivity based cloning technique usually results in an increase in Client throughput, however we actually see a decrease in at the sixth stage. One should note that the sensitivity calculation is based on a small change to input parameters. However, by cloning S4 from 1 to 2, the number of clones are increased by 100% which is too large for the approach to predict.

4 CONCLUSIONS

In this paper an approach for determining sensitivities of distributed applications models was presented. The approach combines the sensitivities of separate queueing networks into one model. Using this approach one is able to determine sensitivities of all model output parameters to model input parameters using only one model solution. The output of the technique is a ranking of the sensitivities. The ranked sensitivities were then used to determine most sensitive parameters and in turn used in improving system performance.

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ON THE USE OF VARIANCE REDUCING MULTIPLIERS IN MONTE CARLO COMPUTATIONS OF A GLOBAL SENSITIVITY INDEX

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1 A NEW VARIANCE REDUCING TECHNIQUE

Recently a new method for decreasing errors in Monte Carlo integrations was proposed — variance reducing multipliers [1]. For constructing such a multiplier one must have an easy reference function $v(x)$ strongly correlated with the integrand $\varphi(x)$; then the variance may be decreased by a factor $1-r^2$ where r is the corresponding correlation coefficient.

The present paper is a report of an attempt to apply multipliers in Monte Carlo estimations of global sensitivity indices [2], also [3,4,5].

2 GLOBAL SENSITIVITY INDICES

Assume that the model under investigation is described by a function $f(x)$, where $x=(x_1,\ldots,x_n)$ and each x_i varies from 0 to 1. All the multidimensional integrals below are from 0 to 1 for each variable.

Denote by y a specified subset of m variables $x_{i_1},\ldots,x_{i_m}$ and let z be the set of $n-m$ complementary variables, so that $x=(y,z)$. We apply the Monte Carlo method for estimating the following four quantities:

$$f_0=\int f(x)dx, \qquad D_y=\int f(x)f(y,z')dxdz'-f_0^2,$$

$$D=\int f^2(x)dx-f_0^2, \qquad D_z=\int f(x)f(y',z)dxdy'-f_0^2.$$

Then the global sensitivity indices for y and z are computed:

$$S_y=D_y/D, \qquad S_z=D_z/D,$$

and

$$S_y^{tot}=1-S_z, \qquad S_{yz}=1-S_y-S_z.$$

We recall that $0\le S_y\le S_y^{tot}\le 1$, and that $S_y=S_y^{tot}=0$ means that $f(x)$ does not depend on y while $S_y=S_y^{tot}=1$ means that $f(x)$ does not depend on z.

3 THE COMPUTATION SCHEME

In order to avoid losses of accuracy, it was recommended in [2] to precompute roughly f_0, and to consider $f(x)-f_0$ instead of $f(x)$. Then the new f_0 will be near to zero. In this situation the variance reducing multiplier is inefficient (as well as several other variance reducing techniques). Therefore we have decided to use one and the same easy function $a(x)$ that is similar to $f(x)$ for setting up three reference functions for computing the integrals in D, D_y, D_z, while f_0 is estimated by crude Monte Carlo. These reference functions are proportional to $a^2(x)$, $a(x)a(y,z')$ and $a(x)a(y',z)$ respectively.

4 FIRST EXPERIMENT

A nonlinear model

$$f(x) = \exp \sum_{i=1}^{n} b_i x_i - I_n + c_0$$

is studied; here

$$I_n = \prod_{i=1}^{n} (e^{b_i} - 1)/b_i$$

and each $0 \le x_i \le 1$. For this model $f_0 = c_0$. However in our experiments the value of f_0 was estimated numerically and the computations confirmed that small variations of c_0, $0 \le c_0 \le 1$, had no influence on the results.

We considered a linear approximating model

$$a(x) = \sum_{i=1}^{n} b_i \left(x_i - \frac{1}{2} \right)$$

For linear functions, only the first order sensitivity indices can be positive.

If the coefficients b_i are small then $a(x) \approx f(x)$ and there is a considerable gain in accuracy due to the variance reduction. However, as a rule, accuracy requirements for sensitivity indices are moderate and in this situation the indices for $f(x)$ and $a(x)$ can be regarded as equal. Hence, this case is not very interesting for SAMO.

On the other hand, if the coefficients b_i are large, there is no similarity between $a(x)$ and $f(x)$, and no variance reduction.

The most interesting is the intermediate case when the b_i-s are neither small nor large: you cannot replace the sensitivity indices for $f(x)$ by indices for $a(x)$; but you can use $a(x)$ for constructing reference functions and thus obtain a reduction of variance.

Here is one of the numerical examples:

$$n = 6, \quad b_1 = 1.5, \quad b_2 = \cdots = b_6 = 0.9, \quad c_0 = 0.$$

Exact values: $S_1 = 0.287$, $S_2 = \cdots = S_6 = 0.106$; if we consider $y = (x_1)$, $z = (x_2, \ldots, x_6)$, then $S_{yz} = 0.109$.

For the linear model: $\widetilde{S}_1 = 0.357$, $\widetilde{S}_2 = \cdots = \widetilde{S}_6 = 0.129$, $\widetilde{S}_{yz} = 0$.

Table 1 below demonstrates the convergence of the results as the number of Monte Carlo trials N increases. The values $S^+_{y,N}$ were computed with multipliers, the values $S_{y,N}$ — without.

Table 1. Convergence of S_y

N	2^8	2^{10}	2^{12}	2^{14}	2^{16}	2^{18}
$S_{y,N}$	0.405	0.331	0.286	0.278	0.284	0.288
$S^+_{y,N}$	0.264	0.295	0.287	0.284	0.286	0.289

One can easily see that even at $N = 2^8$ the error in $S^+_{y,N}$ does not exceed 10%, while for $S_{y,N}$ the error at $N = 2^{10}$ is still worse.

5 SECOND EXPERIMENT

Consider the Ishigami model function [6]:

$$f(X_1, X_2, X_3) = \sin X_1 + A \sin^2 X_2 + B X_3^3 \sin X_1$$

where X_1, X_2, X_3 are independent random variables uniformly distributed in the interval $-\pi < x < \pi$. The main peculiarity of the model is the dependence on X_3: the first order sensitivity index $S_3 = 0$ however S_3^{tot} cannot be neglected (in the following numerical example S_3^{tot} is almost 10%).

We have selected an approximation that does not depend on X_3:

$$a(X_1, X_2) = C \sin X_1 + A w(X_2),$$

where $C = 1 + 0.2B\pi^4$ and

$$w(x) = \begin{cases} 4\left|\frac{x}{\pi}\right|^2 - \frac{1}{3} & \text{for} \quad |x| \le \frac{\pi}{2}, \\ 4\left(1 - \left|\frac{x}{\pi}\right|\right)^2 - \frac{1}{3} & \text{for} \quad \frac{\pi}{2} \le |x| < \pi. \end{cases}$$

We have introduced three auxiliary functions a_1, a_2 and a_{sq} that were proportional to $a(x_1, x_2)\, a(x_1, x_2')$, $a(x_1, x_2)\, a(x_1', x_2)$ and $a^2(x_1, x_2)$. They were used as reference functions twice:
a_1 — for $f(x_1, x_2, x_3)\, f(x_1, x_2', x_3')$ and $f(x_1, x_2, x_3)\, f(x_1, x_2', x_3)$,
a_2 — for $f(x_1, x_2, x_3)\, f(x_1', x_2, x_3')$ and $f(x_1, x_2, x_3)\, f(x_1', x_2, x_3)$,
a_{sq} — for $f^2(x_1, x_2, x_3)$ and $f(x_1, x_2, x_3)\, f(x_1, x_2, x_3')$.
The integrands $f(x_1, x_2, x_3)$ and $f(x_1, x_2, x_3)\, f(x_1', x_2', x_3)$ were integrated without multipliers.

Here is one of the numerical examples: A=7, B=0.05.
Exact values: S_1=0.219, S_2=0.687, S_3=0; S_{12}=0, S_{13}=0.095, S_{23}=0, S_{123}=0.
For the approximate model: $\widetilde{S}_1$=0.309, $\widetilde{S}_2$=0.691, $\widetilde{S}_3$=0; $\widetilde{S}_{12}$=$\widetilde{S}_{13}$=$\widetilde{S}_{23}$ =$\widetilde{S}_{123}$=0.
Table 2 below is similar to Table 1 and demonstrates the convergence of S_1.

Table 2. Convergence of S_1

N	2^5	2^7	2^9	2^{11}	2^{13}	2^{15}
$S_{1,N}$	0.508	0.296	0.264	0.261	0.221	0.223
$S_{1,N}^{+}$	0.215	0.251	0.261	0.247	0.226	0.223

At small N, values $S_{1,N}^{+}$ are much better than $S_{1,N}$ but as N increases both converge to S_1 and the errors are alike.

In this example, for various integrands and their reference functions correlation coefficients vary from 0.67 to 0.85.

6 QUASI-MONTE CARLO COMPUTATIONS

Turning to quasi-Monte Carlo greatly improves the results when the number of variables is not too large [7]. However the influence of variance reducing multipliers seems less significant because the accuracy requirements are moderate. This may be illustrated by Table 3 that is an analogue of Table 2 (quasirandom Sobol sequences were used).

Table 3. Quasi-Monte Carlo convergence of S_1

N	2^5	2^7	2^9	2^{11}	2^{13}	2^{15}
$S_{1,N}$	0.273	0.203	0.226	0.224	0.218	0.219
$S^+_{1,N}$	0.182	0.196	0.221	0.221	0.218	0.219

And a final remark: theoretically, variance reducing multipliers guarantee the reduction of variance only for large enough N.

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LOCAL SENSITIVITY ANALYSIS OF MEDITERRANEAN SEA TROPHIC CHAINS.

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1 INTRODUCTION

Physical, chemical and biological components are equally important in defining the properties of ecosystems as complex as the marine one. In fact, transport processes can deeply influence biological evolution, by creating spatial structures and affecting the rate of the transformation processes. For this reason numerical models, and especially three-dimensional simulations of the interplay between physical and ecological processes on a basin-wide scale, are nowadays an irreplaceable tool for a new understanding of the dynamic of these ecosystems, based on the integration of different disciplines. In fact, only this approach can explain the time evolution of spatial patterns observed in ecosystems, such as the one originated by the seasonal and interannual variabilities in the first trophic levels.

Because of its reduced space and time scale, if compared with the oceans, the Mediterranean Sea, represents a "natural laboratory", which is worth studying and can act as a sensitive indicator of ongoing global climatic changes. In spite of this, up to now, few comprehensive studies have been focused on it. The present study stems from a previous work, which was aimed at developing an aggregated trophic model (Nutrient-Plankton-Detritus), connected to a general circulation model of the Mediterranean Sea [1]. Realistic simulations were obtained when the external forcings strongly limited and/or perturbed primary producers, and the comparison of simulated distributions with available data sets of nutrients and chlorophyll, led to a corroboration of the model [2]. Nevertheless, even though this trophic submodel is well-behaved in terms of initial conditions and choice of parameters, it will be improved in order to explain some experimental facts, such as the east-west N/P ratio skewness, which is higher in the eastern basin, the growth limitaton in terms of different nutrients in different basins and the higher trophic chains in relation to primary producers.

2 THE TROPHIC SUBMODEL

Analysis of the existing data and a survey of the current literature have suggested the inclusion in the model of two trophic chains: one based on phytoplankton and zooplankton and the other on the decomposition of organic detritus. Nitrogen and Phosphorous are both taken into account as potentially limiting nutrients. Two different species of primary producers are considered: the first is representative of the large diatomes, and the second of the small autotrophic micro-flagellates. Both phytoplanktonic species compete for the same resources, namely nutrients and light, and are grazed by a unique pool of predators.

The detritus chain describes the remaining part of the biogeochemical cycles of carbon and macronutrients, that is the degradation of particulate and dissolved non-living organic matter, which is introduced by exogenous input and is produced within the system by the processes of mortality, excretion and exudation.

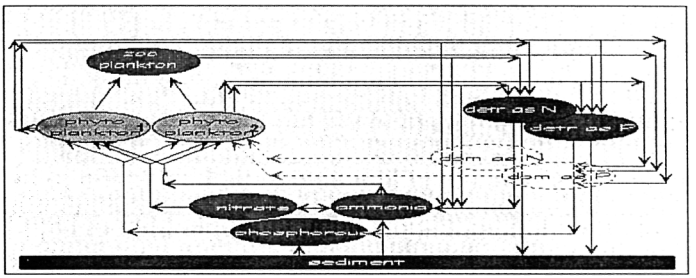
Biological activity is forced by light and temperature, which vary according with seasonal and night/day cycles. The model also take into account self-shading effects, and simulates the variation of the length of the day. The dynamics of Dissolved Oxygen is also reproduced, since this variable, besides being frequently sampled, is an aggregated index of the quality of a water body.

3 LOCAL SENSITIVITY ANALYSIS

The upscaling of the model to a more complex structure calls for preliminary studies, such as an analysis of its stability in specific regions of the space of parameters and a sensitivity analysis of model output. For example, in this case, the parametrization of competition phenomena requires great attention, since slight modifications of the parameters which describe grazing activity, or phytoplankton growth can

change the asyntotic behaviour of the model from the coexistence to the competitive exclusion, which leads to the extinction of one of the two primary producers [3, 4].

Sensitivity analysis, besides giving a first idea of the structural stability of the system around a particular set of parameter values, helps one to in verify that the model is properly designed, i.e. that the selected parametrization is not too detailed in comparison with the available experimental information, because it indicates which parameters are strongly correlated and, therefore, cannot be calibrated against the same data set. Moreover, this technique illustrates the relations between biological and physical processes.



As a first step, in this paper, a local sensitivity analysis of a 1-D vertical model is discussed. The model here presented describes the behaviour of a water column that can be thought of as a part of the integration domain of the full model: Fig. 1 gives a pictorial representation of the link between the state variables at each level. Transport processes within the column are forced realistically, taking into account sinking and diffusion. The 1D model is driven by the same energetic input, light intensity at the surface and temperature along the water column, as is used in the 3D one for forcing the dynamic of the Tirrenian sea. The seasonal evolution of temperature profiles is the one computed with the full 3D model and therefore takes into account also the advection.

Local sensitivity analysis, being based on the linearization of the trajectory of the model, is not as powerful as a global analysis, which allows one to scan a wide region of the space of the input parameters and to deal with model nonlinearites and parameter correlations. Nevertheless, it is computationally convenient, and might be the only way of gaining some insight into the model dynamic when studying large and computationally expensive models. Therefore, with a view to extending the analysis to the whole three-dimensional model of the Mediterranean sea, it has been decided to also apply this method to the submodel here presented. The analysis is developed by using the so-called direct method [5], which was found to be readily applicable to a 1D model of an eutrophic basin [6]. The direct method will be applied to the following vector equation:

$$\partial c/\partial t = \nabla^2 c + f(c,p) \qquad (1)$$

The nominal trajectory of the model correctly reproduces the formation of the well known «deep chlorophyll maximum», as can be seen in Fig. 2. In fact, the dynamic of the primary production is first triggered by light and temperature, and therefore the model shows a bloom of diatoms in the early spring, followed by a bloom of micro-flagellates, which reach their maximum productivity at a higher level of light intensity and temperature. Such blooms cause a rapid depletion of nutrients, which is more pronounced near the surface, where light intensity is higher. Grazing activity starts affecting the phytoplanktonic stocks toward the end of the spring.

Results of the sensitivity analysis are summarized by the PCA analysis of the matrix $\mathbf{s}^T\mathbf{s}$, where $\mathbf{s}$ is the normalized local concentration sensitivity [7]. Such analysis reveals the groups of parameters whose sensitivities are strongly correlated, and which are therefore not identifiable by calibrating the model versus a given data set. This information is extremely important because one can obtain a reliable estimate for only one parameter for each group. In this case, groups of strongly correlated parameters, which have a load above 0.7 in a given eigenvector, are reported in Tab. 1.

The analysis has been performed in the hypothesis of daily samples of Nutrients (concentrations of ammonia, nitrate and ortophosphate), Chlorophill and Dissolved Oxygen, collected at three different depths, namely 5, 50 and 100 meters for one year. In fact, it is necessary to sample these state variables along the

Table 1. Groups of parameters whose sensitivities are strongly correlated and which are not identifiable by calibrating the model versus a given data set. Within each group, the parameter are sorted by decreasing tuning importance.

Group 1	Group 2	Group 3	Group 4	Group 5
Explained variance at superficial, middle and bottom layer. Cumulative varaince is reported between parenthesis.				
34 %	30 (64)	15 (79)	8 (87)	3 (90)
32 %	22 (54)	22 (76)	8 (84)	2 (86)
42 %	24 (66)	20 (86)	3 (90)	--------
Parameters sorted by decreasing tuning importance				
T opt. 2	T opt. 1	Arrhenius coefficient*	Shading coeff. Diatoms §	Ksno1 $
T inib. 2	T inib. 1	Preferential grazing coefficient §	Shading coeff. Flagellates §	Nitrification rate
Max growth rate 2	Max growth rate 1	Max grazing rate §	Shading coeff. Detr§	
Mortality rate 2	Mortality rate 1	Grazer metabolic efficiency 1 §		
T growth coeff 2	T growth coeff. 1	Grazing semisaturation §		
shading coeff water				
I opt 2		Decay rate detr. N#		
I opt 1		Grazer motality rate§		
Ammonia semisaturation 2	Ammonia semisaturation 1	Grazer metabolic efficiency 2 §		
Nitrate semisaturation 2		Sinking rate detritus §		
Phosphate semisaturation 2	Phosphate semisaturation 1			
Inib. Ammonia-Nitrate 2				
Inib. Ammonia-Nitrate 1 +				
Decay rate detritus P §				
Respiration rate 2	Respiration rate 1			
Exudation rate 2	Exudation rate 1			
Sinking rate detr.*				

* only for the data collected at 100 meters depth. § only for the data collected at 5 and 50 meters depths.
+ only for the data collected at 50 meters depth # only for the data collected at 50 and 100 meters depth.
$ only for the data collected at 5 meters depth.

water column because as shown in fig.2, model output is very sensitive to the depth and therefore one should expect that at different depth, dynamic is mainly affected by different subset of parameters.

In summary, model output is less sensitive at the lower layer about biological processes, since there plankton activity is almost null. Instead, at the surface and intermediate layers, a clear distinction appears among parameters referring to diatoms, flagellates and zooplankton. On the basis of the data set hypothesized, 4 or 5 parameters can be calibrated at each level, preferably to be chosen from the ones of greater tuning importance (see below) and keeping in mind that is not possible to identify more than one parameter for each group.

Results indicate that:
1) The parameters with the highest tuning importance are :
- Temperature related parameters (Topt1, Topt2, Arrhenius coefficient, and at a smaller degree T inib.1 and T inib.2)

- Phytoplankton growth (max gr. rate 1 and max gr. rate 2) and mortality (mort. rate 1 and mort. rate 2) parameters
- Grazing activity (max grazing rate and preferential grazing coefficient)
- Water shading coefficient.

2) Even if chlorophill measuraments are data which integrate the biomass of both producers, parameters referring to the two different pools of phytoplankton fall into two distinct groups, and there exists the possibility of calibrating at least one parameter for each pool. The separation, sharper in the superficial and intermediate layer is still present, but less clear, also at the bottom layer, where plankton activity is much more reduced.

3) Parameters related to zooplankton activity are grouped together in the 3rd factor of the PCA, which still explains a significant fraction of the total variance. In the bottom layer, where zooplankton activity is extremely low, these parameters are instead mixed with those related to phytoplankton in the 1st factor, which explains a greater fraction of variance. In this case, the 3rd factor is dominated by Arrhenius coefficient.

4) Light attenuation coefficient due to phytoplankton and detritus have correlated sensitivities, and have the highest loadings in the 4th factor (8% of total variance). Water shading coefficient is instead correlated to the parameters of the 1st factor.

5) The sensitivity of sinking rate of detritus is inversely correlated to grazing activity

6)Whereas the mineralization rate of Phosporous in detritus has a significant effect only at the surface layer, the mineralization of Nitrogen, which is slower, is significant at the intermediate layer (3rd factor, inversely correlated to the sinking and correlated to grazing activity) and at the bottom layer.

7) Nitrification terms have the highest loadings in the 5th factor, if PCA analysis is performed at a depth of 50 meters.

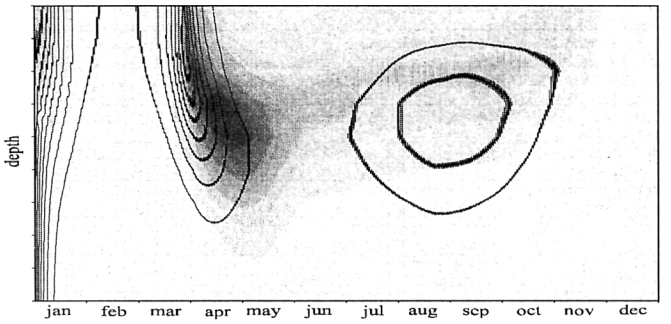


Fig.2. Yearly evolution of diatoms (contour) and microflagellates (shaded) densities along the column

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GLOBAL SENSITIVITY ANALYSIS: AN APPLICATION TO THE EUROPEAN RISK RANKING METHOD (EURAM) FOR EVALUATING HAZARDOUS CHEMICALS

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1 INTRODUCTION

There is a large number of chemicals currently in use in the world. In the European Union (EU) alone, there are 100,195 so-called existing substances (i.e. substances which were deemed to be on the European market before September 18, 1981 and listed in the European INventory of Existing Commercial Substances (EINECS)). In order to provide a legal framework within the EU for the evaluation of existing chemicals, i.e. EINECS substances, Council Regulation (EEC) 793/93 [1] was adopted, in which the evaluation of the existing chemicals is carried out in four steps, namely data collection, priority setting, risk and, if necessary, risk reduction. To fulfil the priority setting step, the EU Risk rAnking Method (EURAM) [2] has been developed to produce rankings which form the basis for drawing up a priority list of substances among the so-called High Production Volume Chemicals (HPVCs), substances produced in the EU in volumes exceeding 1000 tons per year and appearing in the International Uniform Chemical Information Database (IUCLID) [3]. EURAM ranks substances on the basis of their potential risk to man and environment by using a simple exposure-effect model, containing human health and environmental effect endpoints as well as exposure factors.

Sensitivity analysis has been performed on the environmental exposure part of the EURAM model. The aim of the sensitivity analysis is to identify the sources of variability of the aquatic exposure (*AEX*) score of a chemical. Results of this analysis will provide information about the ranking model as part of meeting three main requirements of the ranking method: that it should be (i) transparent, (ii) generally acceptable and (iii) scientifically sound. The analysis can be a guidance for reducing the overall uncertainty of the scores (i.e. greater accuracy of the rankings of the chemicals) by identifying the most influential factors. Furthermore, the analysis may help to group the chemicals according to general characteristics and physico-chemical properties.

In the next section, we present the model, and in Section 3, we describe briefly the sensitivity technique used in the analysis. In the final section we present our findings and give our conclusions.

2 DESCRIPTION OF THE EURAM MODEL

The aquatic exposure score of a chemical is calculated by using a simple exposure model, which include three main factors, namely

- the emissions, based on use patterns and tonnage produced or imported,
- environmental distribution, based on a Mackay level I model [4],
- degradation, based on aquatic biodegradation.

The model for computing the *AEX* score is given by

$$AEX = c_1 \times (\log(P) + \log(\alpha) + \log(\beta) + c_2) \quad (1)$$

where

- P denotes production volume/use pattern and is given by $P = 0.01 \times T_I + 0.1 \times T_{II} + 0.2 \times T_{III} + T_{IV}$, in which T_I is a measure of the tons produced being used in closed systems, T_{II}, tons produced included into or onto a matrix, T_{III}, tons produced for non-dispersive use, and T_{IV}, tons produced for wide dispersive use,
- α represents the MacKay level I model given by $\alpha = [0.205 \times (VP/WS) + 1 + 0.000906 \times K_{ow}]^{-1}$ where VP is the vapour pressure measured in Pa, WS is the water solubility measured in mol/m^3, and K_{ow} is the octanol-water partition coefficient (in this paper $\log_{10}(K_{ow})$ is used and is denoted by LK),
- β denotes the biodegradation parameter which takes the values 0.1 if the chemical is readily biodegradable, 0.5 if the chemical is inherently biodegradable, and 1.0 if the chemical is persistent, and
- c_1, c_2 are normalising constants.

In the model, given by (1), the constants c_1 and c_2 are set to 0.137 and 1.301 so that the AEX score takes a value between 0 and 10, inclusive. The factors we consider are P, WS, VP, LK, and β. Here, the values of WS, VP, LK, and T_I, T_{II}, T_{III}, and T_{IV}, determining the value of P, and β are measured factors. However, β differs from the others in being measured on a discrete scale. All the values are available from the IUCLID database.

3 THE SENSITIVITY ANALYSIS

The sensitivity measures used, the Sobol' sensitivity indices [5], partition the variance of the model output according to sources of variability. The technique is well-documented [6] (see also this Proceedings [7] and [8]) and uses the sampling scheme of Sobol' LP_τ quasi-random numbers [9]. The two types of indices, which measure the effects of a given factor on the output, are the first order indices, S_i, and the total indices, TS_i. The first order ("main effect") sensitivity index is a measure of the variability of the output due to factor i, whereas the total ("total effect") sensitivity index is a measure of the variability of the output due to factor i and all the interactions between factor i and any other factors.

As a preliminary analysis, six chemicals have been selected from IUCLID. For a given chemical, the IUCLID database contains information about the minimum and maximum values of each factor. As there is little knowledge about the likely distribution of each factor, we assume they all follow a uniform distribution between the minimum and maximum values. Sensitivity analysis is performed for each of the chemicals by estimating both indices for all factors.

4 RESULTS AND CONCLUSIONS

First of all, results of the global sensitivity analysis give that, for all six chemicals, first order indices are identical to total ones, which suggests that there are no interactions between the factors. The total sensitivity indices for the six chemicals are shown in Figure 1. Each bar illustrates the partition of the output variance according to the five input factors.

From the analysis, it can be concluded that for chemicals 3, 4, 5 and 6, the main contributor to the variability of the AEX score is the biodegradation factor. However, for chemicals 1 and 2, the source of variability is split between the biodegradation factor and the emissions. It seems that chemicals 1 and 2 differ from the other chemicals in that they are less biodegradable, as the β value for these two chemicals is either 0.5 or 1.0. It is not surprising that the variability of the output is highly influenced by the production volume only for these two chemicals.

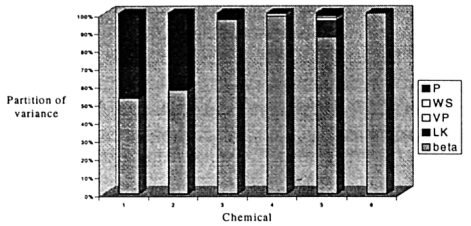

Figure 1: Partition of the variance of the *AEX* score for the six chemicals

Results of this analysis indicate that the investigators who produce the priority list should pay extra attention to how a chemical is classified as biodegradable, as the main source of uncertainty of a score is the biodegradation factor. The results also suggest that the chemicals should be viewed more carefully and possibly be divided into groups of chemicals that have similar features. This could be carried out by investigating the sensitivity of the score of more chemicals, grouping them and for each group determining the more important factors.

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IMPLEMENTATION OF SENSITIVITY CALCULATIONS IN A GENERAL-PURPOSE SIMULATION PROGRAM.

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1 INTRODUCTION

This paper describes the practical implementation of sensitivity calculations in the general purpose simulation program ESACAP [1]. It will also show typically sensitivity analysis of physical systems. ESACAP carries out simulations on non-linear dynamic systems in the time domain and on linear or linearized systems in the frequency domain.

2 SENSITIVITIES IN THE TIME DOMAIN

Exact derivatives of results with respect to parameters are normally computed by means of the so-called sensitivity network [2]. The method is best illustrated by a simple first order integration method.

Consider a non-linear differential algebraic system

$$F(t, V, \dot{V}, \alpha) = 0 \tag{1}$$

defined by a vector of parameters α

This system can be solved by numerical integration. In order to simplify the explanation, consider a first-order method with steplength h. At step n, we have

$$F(t_n, V_n, (V_n - V_{n-1})/h, \alpha) = 0$$

The solution to the non-linear system is obtained by an iterative application of

$$V_n^{(m)} = V_n^{(m-1)} - M^{-1} F(t_n, V_n^{(m-1)}, (V_n^{(m-1)} - V_{n-1}^{(m-1)})/h, \alpha)$$

where m denotes the mth iteration of the non-linear equation solver. M is the Jacobian matrix:

$$M = \frac{\delta F}{\delta V_n} + \frac{1}{h}\frac{\delta F}{\delta \dot{V}_n}$$

A sensitivity vector can be defined as $Z = \frac{\delta V}{\delta \alpha_i}$, i.e. the derivatives of all system variables with respect to the ith element of the parameter vector α_i. It can be found by integration of (1):

$$\frac{\delta F}{\delta V} Z + \frac{\delta F}{\delta \dot{V}} \dot{Z} + \frac{\delta F}{\delta \alpha_i} = 0$$

Again, using a first-order method, we obtain

$$\frac{\delta F}{\delta V_n} Z_n + \frac{\delta F}{\delta \dot{V}_n} (Z_n - Z_{n-1}) / h + \frac{\delta F}{\delta \alpha_i} = 0$$

i.e.

$$\left[\frac{\delta F}{\delta V_n} + \frac{1}{h} \frac{\delta F}{\delta \dot{V}_n} \right] Z_n = - \frac{\delta F}{\delta \alpha_i} + \frac{1}{h} \frac{\delta F}{\delta V_n} Z_{n-1}$$

It is seen that the coefficient to Z_n is M i.e. the Jacobian already available. It is available even in factorized form. Therefore, the additional computational effort for each sensitivity parameter is just one evaluation and substitution of a new right-hand vector.

The method has been implemented into the ESACAP simulation program. ESACAP uses backward-differentiation formulas (BDF) with variable step and order (from 1 to 6) [3]. The paper will demonstrate that the outlined method, can be implemented in a BDF scheme where even the BDF coefficients can be re-used.

3 FREQUENCY DOMAIN

A frequency domain analysis is a so-called small-signal analysis where the response of a linear or linearized system is found. A linearized system may be a result of steady state analysis on a non-linear system. The admittance matrix of the linearized system is found as the last Jacobian before convergence and the linearized system takes the form:

$$YV = J \tag{2}$$

where $Y = G + sC$

G and C are contributions from resistive and reactive elements respectively. The complex variable $s = j\omega$ is inserted and the solution vector V is complex.

Adjoint network theory [2] is used and provides the sensitivity of a certain output with respect to all elements in the coefficient matrix Y.

The interesting fact about the adjoint network approach is the small amount of computational effort required for computing the derivatives of a single output with respect to all parameters. The method requires one single substitution of a simple right-hand vector into a linear system which is the transpose of the admittance matrix i.e.

$$Y^t \hat{V} = A \tag{3}$$

where A is a vector consisting of zeros except for a 1 and -1 at the locations corresponding to the node numberings of the output port. The sensitivity of the output with respect to the branch admittance connected from node i to j is calculated as

$$\frac{\delta V_{out}}{\delta y^{(i,j)}} = -\left(V_i - V_j\right)\left(\hat{V}_i - \hat{V}_j\right)$$

The description language of ESACAP is very powerful. It converts any arithmetic expression specified by the user into postfix code. An interpreter handles the postfix code and provides, besides the results of an expression evaluation, all the partial derivatives required for the building of the Jacobian or for the sensitivities. These derivatives are combined with the adjoint network sensitivities by means of the chain rule.

Frequency domain analysis is mainly used in the analysis of electronic systems such as filters and amplifiers. Recently, a growing interest in other disciplines has shown up, especially in the analysis of dynamic models where a great amount of information can be obtained by comparing frequency domain transfer functions of models with those obtained from experimental data [4].

Frequency domain analysis are also important in the design of control systems. Control systems are found in all engineering disciplines. Stability analyses are carried out by observing the gain and phase vs. frequency of transfer functions or by computing the poles and zeros of these transfer functions. The paper will show how the sensitivity of poles and zeros can be computed.

In communication systems it is important to reduce distortion of the signals. The so-called group delay is a useful tool to describe phase distortion in a communication channel. The group delay is the propagation time for the energy through the system. Therefore, the group delay should be constant over the communication bandwidth. The paper will demonstrate how the group delay is computed as the sum of the sensitivities of all reactive elements in the system. It will also be shown how a particular application of the adjoint network can be used to calculate the sensitivity of the group delay with respect to all parameters.

4 FUTURE WORK

The calculation of sensitivity with respect to all parameters for a number of interesting outputs has been implemented in a general purpose simulator. The next step will be to include these sensitivity calculations into efficient optimisation loops based on gradient methods. Optimisation algorithms are important tools in many engineering activities such as

- Design optimisation
- Parameter identification
- True worst-case analysis

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THE NEED FOR UNCERTAINTY AND SENSITIVITY ANALYSIS IN INTEGRATED ENVIRONMENTAL ASSESSMENT

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1 INTRODUCTION

The environmentally conscious decisions maker, whether politician, business executive or householder, is increasingly facing more and more complex choices. As our understanding of environmental problems increases and their degree of interconnectedness, not only with themselves but also with the socio-economic dimensions of life, becomes more and more apparent, so the decisions over what to do, the scope for action, and the degree of possible effect that different courses of action might have, become increasingly difficult to understand. In this situation there is a clear need for objective "integrated" assessments as a basis and support for sound decision. However, as evidenced by recent cases from Brent Spar to BSE/"Mad Cow" disease, engaging the policy maker and the public with science based information is not as straight forward or as simple as it appears.

While there is a trend towards performing more sophisticated "integrated" assessments in order to obtain a fuller more interconnected picture of environmental problems, so policy makers are increasingly being faced with more complex decisions which can affect domains beyond their particular areas of responsibility. This broadening of the scope of necessary action can lead to a desirable integration of environment into several policy fields. However, the often complex negotiations required to carry this off successfully between the different responsible ministries and stakeholders can instead result in delay or paralysis in decision making and greater unpredictability. This often leads to simplification in order to spur action, which might tackle the short-term immediate causes but not the long-term consequences.

How then to take decisions under conditions of complexity, without simplifying the world too much, and how to equip the analyst, the policy maker, and all those involved in decision making, with the right tools for the job for understanding the problems at the right level of complexity for determining the most efficient and effective policies? Many tools and skills are required for this process. This paper examines the use of Integrated Environmental Assessment (IEA) and in particular the role of uncertainty and sensitivity analysis in IEA for increasing the information value and effectiveness of environmental assessments in a policy context. Written from the point of view of one developing integrated environmental assessments to support policy development and implementation, the paper tries to close the gap between practitioners of uncertainty and sensitivity analysis and those needing to use and apply their results. The paper argues that properly applied in a number of different areas IEA with uncertainty and sensitivity analysis can offer important additional guidance for policy makers; indeed with the uncertainties that will always be present in environmental assessments and the complexities of the problems at stake, the lack of uncertainty and sensitivity analysis in IEAs can be a severe handicap to decision makers using assessment results. The use of such assessments and analysis techniques in a policy context requires, however, a strong commitment, co-operation and understanding from all parties. The practitioner needs to provide the right techniques which are easy to understand and feasible to apply. The policy maker in turn must be prepared to use a new type of information and open the policy making process to critical and transparent appraisal. Without confusing roles this can lead to a new level of co-operation and decision making. As long as uncertainty and sensitivity analysis are left out of policy relevant assessment, scientific based information will never fulfil its full potential as a sound basis for decision making, state of the environment reports and IEAs will remain largely ineffective marginal tools in the policy making process, and the path to sustainable development will remain as unnavigable as ever.

2 PAST PROGRESS

Over the past 25 years there has been much progress in EU countries tackling the causes of well defined environmental problems such as chronic air and water pollution [1]. In particular, those problems with well defined pollution sources of local origin were most easy to tackle where the information was relatively easy to assess, cause and effect established, and courses for action seemed obvious. However, the solutions to these problems, such as raising the height of smoke stacks, led in many cases to intensifying regional-scale problems, such as acidification. Over the last 10 to 15 years, more sophisticated assessment methodologies have been brought to bear on these problems (such as the critical loads concept) to provide a more holistic understanding and response to the problems. Considerable achievements in emission reductions have followed these assessments, but success is incomplete [2] and while new emissions threaten to overturn the successes of the past (such as from the rising emissions from the transport sector) new and more complex problems are emerging (eg, threats to biodiversity, urban-rural sustainability, agriculture and food safety and chemicals in the environment) which have increasingly broad consequences for sectorial policies outside the environmental arena *per se* and for which ever more complex and insightful understanding and courageous decision making is needed if the successes of the past are to be repeated. At the level of sustainable development we are hardly equipped at all with the tools to analyse, let alone to tackle, such problems.

3 PRESENT DILEMMAS

In all fields, good decision making requires good and ideally complete information. Some decisions however need making in the absence of both. In the environmental field, the time constants of processes effecting both the onset of effects and recovery, particularly when some processes are irreversible, often dictate that decisions must be taken sooner rather than later, and that precautionary action is essential. A good decision under such circumstances means making the best of existing information. But what is the best and what is sufficient? How can we increase the information value of existing data?

For some problems, there is time and scope to make more research or data collection, but a limit is always reached. Part of this arises from the unpredictable nature of many environment processes, but part comes from the often unquantifiable values and preferences which define the societies and the politics in which we live, in which we exercise our decisions and which are inextricably linked to many environmental issues. When faced with real policy issues it is therefore necessary to tackle environmental problems together with the socio-economic concerns and consequences in order to obtain effective results. For this there is no ideal fully quantified data set on which to base decisions.

Ravetz [3] expresses this situation as *"decision making under inadequate certainty"*. He notes that decision makers, when engaged on a science-related issue come across this problem when, typically, *"facts are uncertain, values in dispute, stakes high and decisions urgent"*. Climate change is a well known example of this type of problem, as are the BSE and Brent Spar crises mentioned above, but the same characteristics are shared by most environmental problems today. It is no longer possible to treat these problems as before as if the objective facts of natural science are "hard" and the subjective values in society and politics are "soft". To quote Ravetz again: *"The science* [of these problems] *is inconclusive and debatable; and the decisions involve contested interests and have grave consequences."* The information needed to tackle these problems is thus broader and contains unquantifiable terms; the interpretations are complex and subject to debate. Under these circumstances it can be difficult to distinguish between "objective information" and "propaganda" offered as the basis for decision making. However, it is imperative that this distinction is made lest the search for a more integrated approach to policy making fails to recognise or even exclude the very additional information it needs. It is in this context that Integrated Environmental Assessment is beginning to play an important role and to which uncertainty and sensitivity analysis can add significant value.

4 INTEGRATED ENVIRONMENTAL ASSESSMENT

Integrated Environmental Assessment is a tool to support policy making. IEA aims to provide a broad framework within which decisions can be made, where interconnectedness of the environment is defined and possible knock-on effects can be assessed. In other words IEA is a technique and a process to better organise relevant and available information about environmental problems to increase effectiveness of decision making and to reduce uncertainties. IEAs are conducted for the very purpose of supporting the framing and implementation of environmental policies

and are therefore by definition policy orientated and destined to be digested and responded to by policy makers. Being a policy driven activity, IEA is incomplete without the involvement and participation of the public and policy maker; indeed all stakeholders of the issues under consideration.

To analyse environmental problems, an integrated model of the environment and its interaction with human activities is required. The EEA has adopted the so-called DPSIR model which describes the interrelationships for any given environmental problem between Driving Forces, Pressures, State, Impact and Responses. Although in the consideration and treatment of different problems unequal emphasis is often given to each of these five interconnected aspects, a full analysis can only be obtained by analysing the whole system. Following this framework allows the significance and uncertainties of the different elements in the system giving rise to the problem to be properly allocated and assessed.

As mentioned above, the problems we are dealing with are those which require action based upon incomplete understanding. To be most effective IEA has to quantify uncertainties and integrate them into the assessment. Moreover, IEA must also provide decision makers with information about the contributions of different factors to the problems at stake and the degree of susceptibility of the problem to possible responses under consideration.

Integrated Environmental Assessment is not only a tool in the process of understanding and appraising a problem, but, most significantly, it provides a transparent framework within which decisions about responses can be discussed and the need for action debated and made convincing. IEA is particularly useful when implementing the precautionary principle [4]. When facts are uncertain and knowledge incomplete it is not sufficient (and sometimes not possible) only to consider what may be termed the "objective evidence" when taking a decision, especially when values are at stake. In these circumstances, the strength of IEA lies in its transparency. As Ravetz puts it: environmental scientists in this situation are *"judged as witnesses giving testimony rather than as oracles delivering truth"*. The competent admission of uncertainty gives strength and credence to their case. The good management of uncertainty provides assurance to those who need convincing of the need for action.

Clearly then, uncertainty and sensitivity analysis are crucial for effective IEA. Despite this, apart from some notable exceptions (see eg, [5]), the experience and application of these techniques in a policy setting are poorly developed and infrequently used. Indeed, they are often viewed with suspicion since they are seen as obfuscating the facts and as an excuse for a lack of objective information which should instead be remedied with, for example, more data collection or research. This leads instead to an under utilisation of "scientific" data in decision making, to a non-systematic use of available information, and eventually to a poor analysis of policy alternatives.

5 SENSITIVITY ANALYSIS IN A POLICY CONTEXT

Two of the most important questions that environmental policy makers need to answer are: what has been the success to date of current policies, and what additional responses are required to tackle expected future developments of environmental problems? In order to answer the second question it is necessary to answer a third question about the reasons for the observed behaviour. The EEA's triennial EU State of the Environment Reports are developed with these questions in mind. The 1995 report [6] was developed in particular to assist the Commission in the revision of the EC's 5th Environmental Action Programme (5EAP) and was therefore designed to be progress oriented. The 1998 report, currently under development, is broader in scope and will be used to consider if new policy initiatives are required in the follow up to the 5EAP. The scope of these reports is very ambitious. By summarising the available information on the environment and socio-economic developments, and by making comparison with political environmental targets, the 1995 report attempted to indicate the degree of progress made towards environmental goals over the previous years. As an integrated environmental assessment the report attempted to answer the three questions above, but was limited due to the scope and nature of the process in which it was developed. The 1998 report will improve on this experience but will still be severely constrained by the available time, resources, appropriate information and expertise.

Three main shortcomings are relevant here: first, the lack of any formal uncertainty or sensitivity assessment on the distance-to-target analysis making it difficult to assess the significance of the gaps or successes noted; second, the difficulty interpreting the trends where the many different reasons for meeting or not meeting a target can be appraised; and third, the lack of information as to the degree of possible influence that new or strengthened policies might have on the problem with the current uncertainties.

These difficulties in answering the above three questions are elaborated further in the paper to demonstrate how uncertainty and sensitivity analyses can add significant value to existing assessments in a policy context and where efforts should be focused in future work.

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IMPROVED PARAMETER ESTIMATION FOR HYDROLOGICAL MODELS USING WEIGHTED OBJECTIVE FUNCTIONS

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In this presentation attention will be given to calibration of hydrological models. We will measure the improvement of parameter estimation by reduction in a weighted object function. Both parameter estimation and choice of the proper objective function are related to parameter optimization, being an important step in the calibration process, where we search for optimal parameter values within a model schematization. Parameter optimization is the search for the best set of parameters for a given model in a given area of land. We will concentrate on cross-validation methods for hydraulic readings, in which we essentially deal with spatially dependent variables.

1 THEORY

A commonly applied objective function equals the sum of squares between the measured g_i and the modelled b_i hydraulic reading:

$$D_{kwad} = \sum_{i=1}^{n} \left[w_i \, (b_i - g_i)^2 \right]$$

where n equals the number of measurements used for calibration, and its equivalent, the average of the absolute values:

$$D_{abs} = \sum_{i=1}^{n} \left| w_i \, (b_i - g_i) \right|$$

The values of w_i specify user defined weights. We compared four ways of selecting weights:

I. Statistical stratification, in which the observations are stratified into k clusters of similar observations on the basis of prior knowledge: homogeneous mapping units, geohydrologial relations, etc.

II. Distance measured by the Euclidean distance between the validation point and the closest observation point. Let for any test point this distance be equal to d_i. Select a value $a > 0$. Then the weight $w_i = (1/D) \cdot d_i^a$, where D is normalisation constant, $D = S_1 d_i^a$.

III. Kriging and spatial variability, where weights are proportional to the square of the prediction error of kriging the value in the *i*th observation points with all the remaining points. Hydraulic readings are predicted with kriging towards individual observation points, *without* using these points - this yields a prediction error e_i. The weights w_i are equal to a function of e_i, e.g., $w_i = |e_i|^a/E$, where E equals a normalization constant $E = S_1 (1/e_i)^a$. Common values for a are 1 (yielding an absolute weight assignment) and 2 (yielding a squared weight assignment). As such the those locations are assigned the largest weights which are spatially the most deviating ones, that is those which deviate most from their surrounding points. In principle both measured and calculated hydraulic readings can be applied.

IV. Combination with observations on a related covariable. Define k groups and determine within each group individual weight v_i. Take one group as a basis, and assign it the weight $w_i = 1$, for example the readings in the first aquifer. Next determine for each group a weight factor such that the mean deviation of 1 measurement unit is equally contributes as a deviation of a single unit which serves as the basic start. For example, 0.3 for hydraulic readings in the second aquifer and 0.00001 for the fluxes so that 1 m difference in hydraulic readings in the first aquifer corresponds to 1/0.3 m in the 2nd aquifer and to 1/0.00001 m^3/d deviation in the amount of discharged outlet water. Each observation is then assigned a weight equal to the product of the group weight and the group factor.

2 CASE STUDY

These procedures were applied in the geohydrological model TRIWACO within a Dutch polder area. We applied the first three procedures in a straightforward way: for objective function I a prior stratification was applied, for objective function II the value of a was set equal to 1, and for objective function III the interpolated measured values were used and a was again set equal to 1. Three more objective functions were defined on the basis of objective function IV. We first applied a statistical stratification, and within each group we use constant values equal to $1/n_i$, being equal to 1/38 to readings in the first aquifer, 1/24 for the 2nd and ½ for the seepage fluxes. Objective function IVa has equal weights for the three groups. Objective function IVb puts an error in the fluxes of 1000 m^3 day^{-1} equal to an error of 1 m of hydraulic reading. Objective function IVc weighs the groups according to reliability of within the groups, being the reciprocal of the mean squared differences in the initial model. We compared the results with those of a reference objective function (all weights are equal).

Table 1: Values for permissivity (m/d) obtained with the first three objective functions

	Values obtained with object functions			
Value to obtain	0	I	II	III
10.0	18.25	16.64	17.90	4.35
12.5	12.32	12.70	12.25	15.29
8.0	7.27	7.47	7.31	4.99

Table 2: Statistical measures of differences between measured and calculated hydraulic readings for the first three objective function, compared with equal weights

	original	0	I	II	III
Mean difference	-0,002	-0,033	-0,025	-0,030	-0,078
Mean absolute difference	0,226	0,214	0,216	0,214	0,237
Mean squared difference	0,109	0,113	0,113	0,113	0,125

First, three permissivity values were estimated (Table 1). We conclude that in particular objective function III yields very different results from the original permissivity, and that a permissivity equal to 10.0 was hard to obtain with all objective functions.

Next, we compared measured and calculated hydraulic heads (Table 2). Use of weights based on prior information improved the objective function, whereas kriging based techniques resulted in less reliable model calculations, which are, though, governed by a few (spatially) outlying observations. We conclude that weights

should be selected in a simple way. Parameter optimization with kriging based procedures gives clearly deviating results, reflecting the spatial dependence between the observations.

For the composed objective functions IVa, IVb and IVc, a distinction into the two aquifers and the seepage fluxes is relevant (Table 3). Objective function IVa yields unrealistic results, whereas IVb and IVc are equally useful. But the differences are large in all three attempts, with objective function IVb giving possibly the best results.

Table 3: Differences in the two aquifers and the seepage fluxes for the three objective functions Iva-IVc, as compared to the original values

	Orig.	IVa	IVb	IVc
Mean difference in aquifer 1	0.032	-0.549	0.022	0.077
Mean difference in aquifer 2	0.050	0.581	0.062	0.048
Mean difference in seepage fluxes	-572	-0.044	92.6	98.3

To summarize and to conclude, a proper use of objective functions, with proper weight specification may yield important information on parameter estimation. In a practical case study interesting results were obtained, showing an improvement when using weights based on prior information. Interesting results are further obtained when combining different variables with appropriate weights.

ADJOINT SENSITIVITY STUDIES IN NUMERICAL MODELING OF THE ATMOSPHERIC CIRCULATION

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Numerical modeling has now become a basic tool for the study of atmospheric dynamics. Numerical models of the atmospheric circulation are computer programs which determine, to the best possible degree of accuracy, the temporal evolution of the flow from specified initial and lateral boundary conditions. These programs are built on discretized formulations of the physical laws that govern the evolution of the flow, namely the laws of conservation of mass, energy and momentum.

Numerous models, based on various approximations, are used for a wide variety of diverse applications, and particularly for weather prediction. The presently most powerful models for numerical weather prediction use as 'prognostic' variables, describing the state of the flow, temperature, moisture, horizontal wind components and surface pressure. These variables are defined over the entire volume of the atmosphere with a horizontal and vertical resolutions of typically 100 km and 1 km respectively. The dimension of the corresponding state vector (*i. e.* the number of independent parameters defining the state of the flow at a given time) lies in the range 10^6-10^7. The increment for temporal integration is about 15 minutes, and half an hour of CPU time is typically necessary on the most powerful present computers for 24 hours of simulation. The best numerical weather forecasts are at present statistically useful up to a range of about 6-7 days.

Other General Circulation Models (GCMs), similar in their basic principles, but with usually a lower spatial resolution, are used for climatological studies of various kinds. Limited-area models, with both smaller horizontal extent and higher resolution, are used for local forecasts and phenomenological studies. Such limited-area models require the specification of appropriate lateral boundary conditions in the course of their temporal integration.

Still other models, also based on similar principles, are used for the study of the oceanic circulation. A significant part of the research done in the large domain of numerical climatology is at present devoted to the development of coupled models of the atmospheric and oceanic circulations. One can also mention the interesting recent extension of numerical modeling to the study of the dynamics of planetary atmospheres, such as the atmospheres of Mars, Venus and Titan.

In this context, one is naturally led to consider problems which involve, under one form or another, the sensitivity of the output of a model with respect to the input. Here are a few typical examples.

a) One wants to determine the actual physical sensitivity of some output parameters to some input parameters. For instance, a major concern is at present the possible effect on climate of the increase of the atmospheric content in greenhouse gases, such as carbon dioxide.

b) One wants to determine the uncertainty on the output resulting from the uncertainty on the input. A typical example is the uncertainty on a weather forecast resulting from the uncertainty on the initial conditions.

c) One wants to determine what, in the input, is at the origin of a particular feature observed in the output. A typical example is the following. A weather forecast has failed in a significant way, for instance in not predicting the rapid deepening of a depression. What was in the input to the forecast (initial conditions, physical parameters) at the origin of that failure?

d) One wants to determine the input in such a way that the output verify some prescribed condition. This situation will normally lead to the solution of an *optimization* problem. A typical example is *variational assimilation* of observations, in which a model is adjusted to a set of observations distributed in time.

A major obstacle for sensitivity studies of this type is the numerical dimension of atmospheric models and the ensuing cost of the numerical integrations. It would for instance be perfectly impossible to explicitly determine the Jacobian of a model, *i. e.* the matrix of partial derivatives of all output parameters with respect to all input parameters. One must be content, when performing sensitivity studies with a numerical model of the atmospheric circulation, with a very small number of explicit integrations of the model. In this respect, the development in the last few years of the *adjoints* of numerical models of the atmospheric circulation has been a major breakthrough, which has made possible many sensitivity and optimization studies whose cost would have otherwise been absolutely prohibitive.

The principle of adjoint (or reverse) differentiation is simple, and has been described in various contexts by many authors (for meteorological or oceanographical applications, see, *e. g.*, (1) or (2)). Adjoint differentiation is based on a systematic use of the chain rule. It allows the explicit computation of the partial derivatives of one (scalar) output parameter of a model with respect to all input parameters at a numerical cost which is typically (and independently of the numerical dimension of the model) two or three times the cost of one direct integration of the model.

In the last ten years or so, adjoint differentiation has been successfully applied to the solution of many problems in dynamical meteorology. One particular application is variational assimilation of observations, already mentioned above, in which a model is adjusted to a set of observations distributed more or less regularly in both space and time. This is achieved by minimization of an appropriate *objective function* measuring the 'distance' between a given model solution and the observations. The control variables with respect to which the minimization is performed are usually chosen to be the initial conditions of the model at the beginning of the time period over which the observations are distributed. The minimization of the objective function is performed through an iterative 'descent' algorithm, each step of which requires the explicit computation of the local gradient of the objective function with respect to the control variables. This gradient is computed by integration of the adjoint model. In spite of the relatively large number of iterations required by the minimization (a few tens typically), variational assimilation looks extremely promising, and is being actively developed in several major meteorological centres with a view to operational implementation (see, *e. g.*, (3)).

The quality of numerical weather forecasts varies very much from one forecast to another. Reference (4) describes a study of the errors in the forecasts produced operationally by the European Centre for Medium-range Weather Forecasts. To that end, they have used the adjoint of the forecasting model to compute the gradient, with respect to the initial conditions of the forecast, of the Northern Hemisphere 2-day forecast error. In the medium-range (5 days), large-scale Northern Hemisphere forecasts are typically correlated with the observed fields to a level of about 75%. Occasionally (once a month or so), the quality of forecasts drops to much lower values. It is shown in reference (4) that, on such occasions, the gradient of the forecast error with respect to the initial conditions tends to concentrate in small geographical areas. In addition, the thermal structure of the atmosphere in those areas corresponds to conditions of high instability, in which slight changes in the initial conditions can result in large changes in the resulting forecast (the particular instability process involved here is the so-called baroclinic instability, which is linked to the presence of a latitudinal gradient of temperature, and is at the origin of the formation of the depressions which govern the weather of middle latitudes). Still more importantly, *a posteriori* correction of the initial conditions in the direction of the computed gradient systematically resulted in improvement of the fit of the ensuing integration to the observed fields. This extended to the 5- to 6-day range, well beyond the 2-day range at which the later observations were used for correcting the initial conditions. These elements are all in agreement with the hypothesis that the occasional relatively large forecast errors of the middle latitudes are due to misspecification of the initial conditions in geographically limited unstable areas.

The *a priori* identification of such unstable areas would of course be extremely useful if it was possible to concentrate observations on those areas. 'Sensitive' areas can actually be determined *a priori*, without any need for waiting for new observations, for instance by computing, again through the adjoint model, the *singular modes* of the model, *i. e.* those directions in which initial perturbations will lead to the most rapid growth of energy (5.6). This has been recently attempted in real time on the occasion of the Front and Atlantic Storm Track Experiment (FASTEX), held over the Northern Atlantic Ocean in January and February 1997. Several numerical models and their adjoints have been used in order to determine particularly sensitive areas, which have then been targeted for additional observations, in the form of sondes dropped by airplanes. Preliminary results, presented at the recent Third Workshop on Adjoint Applications in Dynamic Meteorology (Lennoxville, Quebec, Canada, June 1997), show the positive impact of such additional observations on the quality of the ensuing forecasts.

The above results, and others, show the efficiency of adjoint sensitivity studies in the broad domain of numerical meteorology. The development of such studies has however been seriously hampered by the cost of merely developing the necessary adjoint codes in the first place. As soon as the value of adjoint models became clearly apparent for dynamical meteorology, procedures were defined for deriving the adjoint of a given code. These consist in linearizing, and then 'transposing', each elementary coding instruction. The transposed instructions are then

connected together, in reversed order, in order to build progressively larger and larger components of the global adjoint code (see (7) for more information on these points). The size of numerical models of the atmospheric circulation is however very large (typically • 10^5 executable statements), and the hand derivation of an adjoint code, even though it is straightforward, is also a very tedious, lengthy, and error-prone task. Two 'adjoint compilers', *i. e.* software modules capable of automatically deriving the adjoint of a given code by transposing each elementary instruction, and then connecting the transposed instructions, have been developed. The ODYSSÉE compiler, developed by Rostaing and collaborators, is described in (8), and the Tangent and Adjoint Model Compiler (TAMC), developed by Giering and Kaminski, is described in (9). Depending on the form of the direct model, the use of these compilers may still require some preliminary work by hand, but they are progressively becoming more and more efficient, and complete adjoint models have now been developed with each of them. The availability of such compilers will greatly help the implementation of sensitivity studies, not only in the fields of dynamic meteorology and oceanography, but in all fields which use large scale numerical modeling. This includes for instance all aspects of numerical modeling of fluid flows.

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ANALYZING THE EFFICIENCY OF QUANTITATIVE MEASURES OF IMPORTANCE: THE IMPROVED FAST

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1 INTRODUCTION

The improved FAST, our latest innovative technique, seems to be very close to the ideal tool for Sensitivity Analysis (SA): in other words, it may be quite reasonably termed as a *global importance measure.*

We agreed to use the term global basically to underline the contrast with the class of local methods, those based on Taylor expansion, otherwise termed methods for differential sensitivity analysis. In several fields, such as design, signal processing or risk analysis, the local techniques are, even today, improperly believed to be the Sensitivity Analysis *per antonomasia.* Actually, some basic features differentiate global from local measures since, for many practical applications, the latter is definitely limitative. First of all, a global measure allows each uncertain factor i) to vary within a non negligible region of interest and ii) to take into account any possible probability distribution. Secondly, when estimating a sensitivity index for a given factor, in a global measure all the other factors are allowed to vary simultaneously, while in a local analysis they are kept constant at a given central (nominal) value. A global measure is therefore closer to the reality, given that uncertainties affect the factors simultaneously, and not one at a time.

From our point of view, some other important features are necessary for a sensitivity analysis method to be termed as *global.* These features may be summarised by a set of keywords. A global sensitivity measure should be simultaneously *quantitative, model independent, agile and computationally efficient.* An exhaustive definition of these terms is given in [1]. However, let us discuss more in detail what we mean by a *quantitative* and *computationally efficient* measure, by referring mainly to our extended FAST.

2 QUANTITATIVE METHODS

In a *quantitative* measure 100% of the output uncertainty is accounted for, being suitably apportioned to all the sources of uncertainty. A quantitative method is therefore capable of appreciating not only the effects of single factors (the so-called first order effects or main effects, as computable by either regression or correlation techniques), but also the influence that interactions among factors, at any order, may have on the output uncertainty. It is important noticing that existing techniques, such as Standardised Regression Coefficients (SRC) or Correlation Ratios, are quantitative only for models being perfectly linear or additive, respectively. On the other hand, the importance measure proposed by [2] — further improved conceptually and computationally by [3] — and the extended FAST introduced in [4] are definitely quantitative, being based on the unicity of the decomposition of the model $f(\mathbf{x})$ into summands of increasing dimensionality

$$f(x_1,\ldots,x_n) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i,x_j) + \ldots + f_{1,2,\ldots,n}(x_1,\ldots,x_n)$$

where all the terms are orthogonal to each other. The variance decomposition scheme [2]

$$D = \sum_{i=1}^{n} D_i + \sum_{1\le i<j\le n} D_{ij} + \ldots + D_{1,2,\ldots,n}$$

can be derived naturally by defining the partial variances as:

$$D_{i_1,\ldots,i_s} = \int_{K^n} f^2_{i_1,\ldots,i_s}(x_1,\ldots,x_s)\,dx_{i_1},\ldots,dx_{i_s}$$

and the total output variance as:

$$D = \int_{K^n} f^2(\mathrm{x})d\mathrm{x} - f_0^2,$$

where K^n represents the domain of the input factors. It is straightforward to introduce the sensitivity indices as follows

$$S_{i_1,\ldots,i_s} = \frac{D_{i_1,\ldots,i_s}}{D} \tag{1}$$

with the important property that all the effects among factors, at any order, are accounted for, and that the indices add up to one exactly, thus accounting for 100% of the output variance.

By using the importance measure proposed by [2,3] one separate sample of size N is needed to evaluate each of the $2^n - 1$ indices given in 1, thus rendering the analysis computationally unsustainable. The usefulness of the *total* index is then clear [3]. A total index is defined as $S_{Ti} = 1 - S_{\sim i}$, where $S_{\sim i}$ is the sum of all the $S_{i_1,\ldots,i_s}$ terms which do not include the index i.

An analysis based on total indices can also be considered as quantitative, since the entire total output variance is still accounted for. Furthermore, it is definitely worth to evaluate both the S_i's and the S_{Ti}'s — only $2*n$ indices are evaluated instead of $2^n - 1$ — in order to investigate the predominance of either additive effects or interactions among the factors.

Both the improved FAST and the measure proposed by [2] and [3] — let us call it the Sobol', Homma and Saltelli (SHS) measure — yield estimates for the S_i's and the S_{Ti}'s. However, the estimates are based on a completely different procedure: the improved FAST evaluates a one-dimensional integral over a suitably defined *ergodic curve* going through the input domain (see [4]), whereas SHS is based on multidimensional integrations over the domain of the input factors.

3 COMPUTATIONALLY EFFICIENT METHODS

The degree of efficiency of a given estimator is the result of the combination of properties belonging to the estimator itself: extensibility, accuracy, consistency and robustness.

Extensibility is the capability of estimating as many quantities as possible with a single sample. It can be noticed that the improved FAST is more extensible than the SHS importance measure by a factor two. Indeed, when using the SHS importance estimators, one separate sample of a given size N is needed to compute each index, be it first order or total effect. In contrast, the improved FAST can yield, by means of a single sample, the couple (S_i, S_{Ti}) for a given factor i. For instance, in a case with n factors, a total of $n * N$ model evaluations will be performed in order to estimate all the S_i's and the S_{Ti}'s by using the improved FAST, whereas the same set of indices may be obtained via the SHS importance measure by doubling the computational effort.

Accuracy is how close the sensitivity estimates are to the true values at a given sample size N. This property for the estimator may influence the computational cost of the analysis, too.

Consistency is to what extent the variance (amplitude of the error-bar) of the estimate tends towards zero as N approaches infinity.

Robustness may be identified with the amplitude of the estimate's error-bar at a given sample size.

We aim to discuss accuracy, consistency and robustness for both the new FAST and the SHS importance measure from the results obtained in an analytical test case as shown in Figures 1 and 2. The test case is based on the Sobol' analytic g-function [5] in the case with 8 factors. Two sets of values for the factors have been selected and are displayed in Table 1 together with the analytical values of the S_i's and the S_{Ti}'s. To investigate the efficiency of the two methods, the experiments have been repeated $N_{rep} = 100$ times for each sample size and for each case. The sample sizes selected in this study are 64, 128, 256, 512 and 1024 for SHS. Similar values (65, 129, 257, 513 and 1025) have been used in the improved FAST, being the sample size constrained via the formula $N = 2M\omega_i + 1$, where M is related to interferences and ω_i is the integer frequency chosen for factor i (for more details see [4]).

Case	a_i	Analytical value of S_i	Analytical value of S_{Ti}
A	{0, 1, 4.5, 9, 99, 99, 99, 99}	$\{.716,\ .179,\ .024,\ 7.16\cdot10^{-3},\ 7.16\cdot10^{-5},\ 7.16\cdot10^{-5},\ 7.16\cdot10^{-5},\ 7.16\cdot10^{-5}\}$	$\{.787,\ .242,\ .034,\ .010,\ 1.05\cdot10^{-4},\ 1.05\cdot10^{-4},\ 1.05\cdot10^{-4},\ 1.05\cdot10^{-4}\}$
B	{99, 0, 9, 0, 99, 4.5, 1, 99}	$\{3.49\cdot10^{-5},\ .349,\ 3.49\cdot10^{-3},\ .349, 3.49\cdot10^{-5},\ .012,\ .087, 3.49\cdot10^{-5}\}$	$\{6.83\cdot10^{-5},\ .512,\ 6.81\cdot10^{-3},\ .512, 6.83\cdot10^{-5},\ .022,\ .158, 6.83\cdot10^{-5}\}$

Table 1: Choice of a_i values for the Sobol' g-function and the corresponding analytical values of First Order and Total Sensitivity Indices for the set of input factors x_i.

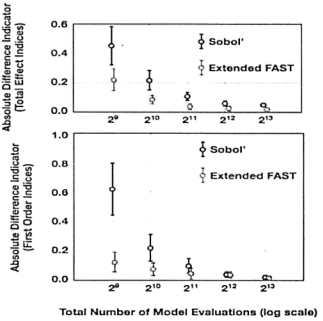

Figure 1: Plot of MAD's and error-bars versus total number of simulations for case A of Table I. The upper figure is related to total effects, the lower one to first order indices

The comparison is based on the Mean Absolute Difference (MAD) indicator, namely

$$MAD = \frac{1}{N_{rep}} \sum_{j=1}^{N_{rep}} \sum_{i=1}^{n} \left| \widehat{S}_{(T)ij} - S_{(T)i} \right|$$

which is plotted in Figures 1 and 2 against the total number of model evaluations involved for computing the whole set of indices. The standard deviations of the mean absolute differences are presented in the figures as error-bars. First of all, it can be noticed that the MAD's for the improved FAST are lower than that for the SHS measure at any sample size, except case B (Figure 2) for the total indices where their values are almost the same. This means that a given accuracy may be obtained with a minor computational effort by expanding the test model in Fourier series evaluated along a one-dimensional curve, rather than using SHS. Secondly, both methods show a decrease in the amplitude of error-bars as N increases, thus meaning that their consistency is quite good. Thirdly, the error bars for FAST seem to be almost everywhere narrower than the corresponding ones for SHS, thus showing a generally better robustness of the improved FAST. From the previous analysis the improved FAST appears to be generally more efficient than SHS: the most convincing piece of evidence is the validity of the *extensibility* property that renders the improved FAST computationally more efficient by at least a factor two.

We wish to make a final remark on the flexibility of the improved FAST compared to that of the original FAST [6]. In classical FAST the sample size is constrained by the formula $N = 2M\omega_{max} + 1$ where ω_{max} is the maximum value within the adopted set of frequencies. A point in favour of classical FAST is that with N simulations the whole set of S_i's can be estimated. On the other hand, a strong disadvantage is that as the number of input factors grows it becomes more and more difficult to avoid interferences among higher harmonics, unless higher and higher values for ω_{max} are selected (according

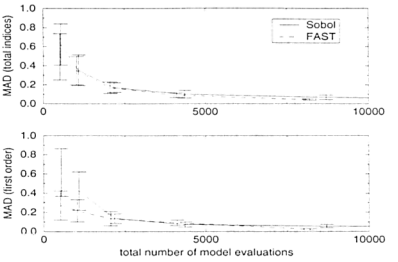

Figure 2: Plot of MAD's and error-bars versus total number of simulations for case B of Table I. The upper figure is related to total effects, the lower one to first order indices

to the algorithm given in [6]). The minimum number of simulations required grows approximately as the square of the number of factors whereas, as depicted above, this relation is linear when extended FAST is employed. In a case with 50 factors, for instance, no less than 43606 simulations are required, and this could be computationally unsustainable (see Table VI at page 1147 of [6]).

In extended FAST a similar relation holds, ie $N = 2M\omega_i + 1$. Given that ω_i is concerned with a single factor only, the problem here is restricted to the interferences between the frequencies pertaining to the evaluation of D_{-i} (the four lowest ones, for instance) and those pertaining to the estimation of D_i. Therefore, whatever the number of factors is, it is always possible to choose $\omega_i = 8$ (see the definition of sets of frequencies free of interferences, given in [6]) and, hence, $N = 65$ (given that, usually, M is set to 4). By referring to the case with 50 factors, the total number of simulations required is restricted to $65x50 = 3250$. Running extended FAST with a total of 3250 simulations would of course lead to a lower accuracy rather than using classical FAST with 43606 simulations. What we wish to strenghten is however the *flexibility* of extended FAST to allow the evaluation of sensitivity indices via a restricted number of model evaluations.

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DEVELOPMENT OF CHEMICAL KINETIC MODELS USING SENSITIVITY ANALYSIS INFORMATION

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1 APPLICATION OF LOCAL SENSITIVITY COEFFICIENTS FOR MECHANISM DEVELOPMENT

Combustion processes are among the most important chemical reactions for human civilization. Even small increase of the efficiency of combustion processes may lead to significant financial savings. Optimization of combustion processes can make then 'greener', decreasing the emission of pollutants that cause global warming and smog. A possible way for such an optimization is based on a full understanding of the chemistry of combustion. The detailed reaction mechanisms used contain several hundred or thousand parameters and therefore sensitivity analysis is of primary importance in this field [1].

A detailed mechanism of 351 irreversible elementary reactions has been created [2] that describes the oxidation of hydrogen, carbon monoxide, methane, ethane, ethylene, and acetylene. The mechanism, called the Leeds Methane Oxidation Mechanism, has been tested against data collected in plug-flow and perfectly stirred reactor experiments, shock tubes, and laminar flame velocity and concentration measurements. Programs of the CHEMKIN package [3] were used for the simulations. Local sensitivities were calculated for all fuels and all reactor types, in each case at fuel lean, stoichiometric, and fuel rich conditions. The normalized local sensitivity coefficient, $\partial \ln Y_i / \partial \ln k_j$, shows the linear effect of changing rate coefficient k_j on simulation result Y_i. In case of laminar flames, flame velocity can be calculated and its sensitivity to a rate coefficient is a unique value for a given cold boundary composition. However, temperature and species concentrations have a spatial profile and the calculated sensitivities also have a spatial profile.

Figure 1 shows three types of sensitivities for a laminar stoichiometric ethane-air flame. Ten reactions are listed in the order of decreasing flame velocity sensitivities. Sensitivities of H atom concentration and of temperature are also given at 1800K, that is near the flame front.

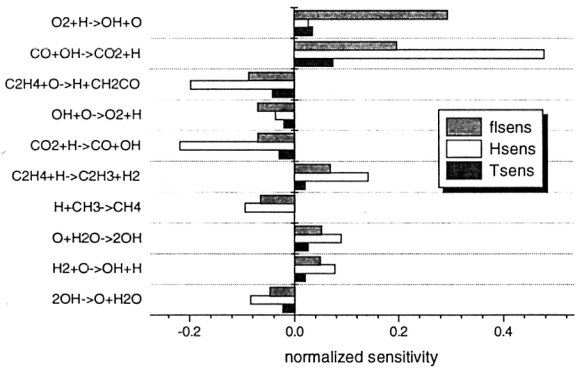

Figure 1. Flame velocity sensitivities (flsens) calculated for a laminar stoichiometric ethane-air flame. Also, H atom concentration and temperature sensitivities are shown at the location of the flame front.

According to Figure 1, the two highest sensitivity reactions are the main chain branching reaction, $O_2+H\rightarrow OH+O$, and the most exothermic reaction $CO+OH\rightarrow CO_2+H$. Surprisingly, no elementary reaction of ethane has a high sensitivity in the ethane-air flame. Spread of the flame front is dictated mainly by the diffusion of H atoms and heat, therefore there is a strong correlation between the flame velocity sensitivities and the H atom concentration and temperature sensitivities calculated at the flame front. In all cases studied, sensitivity coefficients provided an insight into the chemistry and physics of the combustion phenomenon simulated.

Each test case can be characterized by the type of the fuel, the reactor, the model output, and the initial concentration set. In each case, 6-8 reactions had much higher sensitivities than that of the rest. This means that the rate coefficients of these reactions have to be known with high precision. All in all, 52 reactions of the total 351 reactions had a high sensitivity in any test case. Note, that many other reactions have to be present in the mechanism, even if knowing the exact value of their rate coefficient is not important.

In the last years, efforts were made to continuously update the Leeds Methane Oxidation Mechanism. Rate coefficients of gas reactions are frequently redetermined by new, more accurate experimental methods. If the newly suggested rate coefficient is not very different from the previous one and it is not among the 52 most important reactions, the mechanism can be updated without a new validation circle. If the new rate coefficient is among the significant ones, the sensitivity tables indicate which test cases have to be recalculated. Application of sensitivity data provides an efficient way for continuously updating detailed mechanisms with manageable efforts.

2 UNCERTAINTY ANALYSIS BASED ON LOCAL SENSITIVITIES

Some of the chemical kinetics databases (*e.g.* [4]) contain numerical information on the uncertainty of rate coefficients. Traditionally, this uncertainty number f is defined as the base ten logarithm of the ratio of the extreme possible value and of the best estimation, that is $f = \log_{10}(k_{max}/k_0)$. Until now, factor f has been used as a background information only or for the calculation of the so called 'combined sensitivity/uncertainty index', which is a semi-quantitative uncertainty measure [5].

We have utilized the uncertainty factor f in a more quantitative way. In our approach, $\ln k$ is assumed to be a stochastic variable with symmetrical pdf and $\ln k_{max}$ is considered [6] to be a 3σ statistical limit. This way, the uncertainty factor f can be converted to the variance of the logarithm of ith rate coefficient $\sigma(\ln k_j)$. Since rate coefficients were determined independently, local sensitivity coefficients can be used [7] for the determination of a linear estimation of the variance of the model output:

$$\sigma_j^2(Y_i)=\left(\frac{\partial Y_i}{\partial \ln k_j}\right)^2 \sigma^2(\ln k_j) \tag{1}$$

$$\sigma^2(Y_i)=\sum_j \sigma_j^2(Y_i) \tag{2}$$

$$S\%_{ij}=\frac{\sigma_j^2(Y_i)}{\sigma^2(Y_i)}\times 100 \tag{3}$$

where $(\partial Y_i/\partial \ln k_j)^2$ is the square of seminormalized sensitivity coefficients, that is $(\partial v/\partial \ln k_j)^2$, $(\partial T/\partial \ln k_j)^2$, or $(\partial c/\partial \ln k_j)^2$, if the calculated output of the model is flame velocity v, temperature T, or concentration vector c, respectively. The square of variance of model output, $\sigma^2(Y_i)$, is the sum of the contributions of the uncertainty of each rate coefficient to model output Y_i, denoted by $\sigma_j^2(Y_i)$. Partial variance $S\%_{ij}$ indicates the percentage contribution of the uncertainty of rate coefficient j to the total uncertainty of model output Y_i.

Uncertainty factors for all reactions of the Leeds Methane Oxidation Mechanism have been collected and program KINALC [8, 1] was extended for the calculation of both the Warnatz' type combined sensitivity/uncertainty indices and the above described variance based uncertainty analysis.

As an example, calculated laminar flame velocity of a stoichiometric ethane-air flame is 45.7 cm/s. The calculated variance of the flame velocity is 5.6 cm/s. Figure 2 shows that reaction $CO+OH\rightarrow CO_2+H$ and reaction $O_2+H\rightarrow OH+O$ have the highest partial variances (38% and 31%, respectively), while the partial variance of all

other reactions is below 5%. These two reactions have also the highest sensitivities, but in reversed order. The reason is that reaction $CO+OH \rightarrow CO_2+H$ is less known (f=0.5) than reaction $O_2+H \rightarrow OH+O$ (f=0.3). Such calculations provide hints, which rate coefficients have to be determined with a higher accuracy for a better characterization of combustion system investigated.

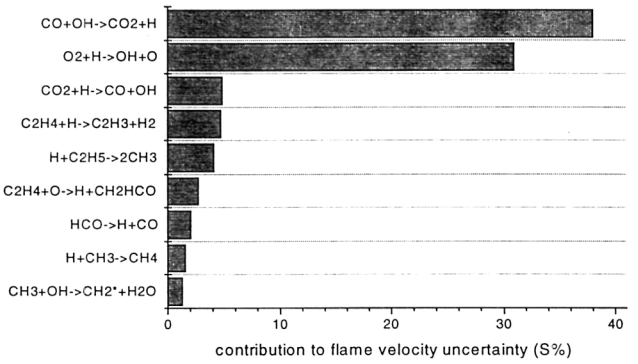

Figure 2. Partial variance S% shows the contribution of the uncertainty of the rate coefficient of each reaction to the uncertainty of the calculated laminar flame velocity for a stoichiometric ethane-air flame.

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MULTI-CRITERIA APPROACH: THE WAY TO DECREASE THE SENSITIVITY OF SOLUTION FROM INPUT PARAMETERS

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1 INTRODUCTION

The optimization problems and optimization algorithms are the essential component of the modern computer mathematics. In reviewing the variety of available algorithms for local and global optimization it is often skipped that in most practical cases we deal with *several* optimization criteria, not with a single merit function. The standard widespread solution is to use the weighted sum of the criteria to produce a single merit function for a single-criteria optimization process.

Unfortunately the naive and presumptuous hope that playing with the weight coefficients enables to investigate the intrinsic multicriteria nature of the problem and to find a reasonable compromise between several inconsistent criteria becomes the truth only for simple model cases. Moreover, the experiments show that very often a smooth change of weights results to abrupt jumps of the weighted optimum in parameter space. Such unexplained jumps, of cource, cannot make the problem under investigation more clear for the User.

Instead of weighted criteria the Pareto set approach to multicriteria optimization [1] should be used. In this case the output of the computer optimization is not the single point of optimum, but the continuous *Pareto set* composed from such points that no criteria can be improved further without making worse some other criteria. Literally saying, the Pareto set approach is based on the paradigma that the computer should optimize the problem as far as the optimization is formalized undoubtedly and that the final solution (the selection of one point from the set of points) should be done by a human expert using non-formalized internal criteria. It will be shown that the Pareto set approach is more stable than the method of weighted criteria, and that it does not obey unstability and abrupt jumps even for non-convex nature of the problem under consideration.

Although the full *continuous* set of points composing the Pareto set cannot be constructed numerically, it is not too difficult to construct a discrete and final *subset* of the Pareto set where the constructed points are more or less dence inside the Pareto set under investigation. A special algorithm *MultiBARS* which generalizes the random-search strategy described in [2, 3], is suggested. The examples of some practical multi-criteria optimization problems using *MultiBARS* and Pareto set ideology, are represented.

2 THE CONCEPT OF MULTI-CRITERIA OPTIMIZATION

Suppose there is some model which is characterized by the variated (i.e., selected by the User) parameters $\vec{x} = (x_1, \ldots, x_n) \in \mathcal{X} \subset R^n$ and the *vector* of criteria $\vec{F} = (f_1(\vec{x}), \ldots, f_s(\vec{x})) \in \mathcal{F} \subset R^s$. The problem under consideration is to find the maximum of $\vec{F}$, where the first problem to be considered is to define what should be implied by a maximum of a vector function.

Let us define the Pareto set $P \subset \mathcal{F}$ of the problem under consideration as the set of such points $\vec{f}^* \in \mathcal{F}$ that for each point $\vec{f} \in \mathcal{F}$ ($\vec{f} \neq \vec{f}^*$) at least for one k the condition $f_k < f_k^*$ is fulfilled [1]. By changing the input parameter $\vec{x}^*$ it is possible to increase some criteria components in $\vec{f}^*$ but it results immediately to decreasing of at least one criterium. We will consider the Pareto set of the problem as the solution of the multicriteria optimization assuming that it is the turn of an expert to select *one* solution from this continuous set when the computer succeeds to find it.

Fig. 1 (a) shows the set $\mathcal{F}$ for some test problem with two criteria f_1 and f_2 and fig. 1 (b) — the corresponding Pareto set P, which is composed from two lines KL and MN. It is not a rare case that for

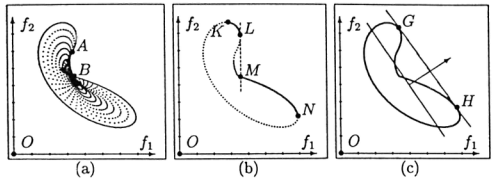

Figure 1: Pareto set for some test problem

smooth and simple problem the set of criteria values is non-convex and that the Pareto set is scattered into several pieces.

The definition of the solution of multi-criteria optimization as the Pareto set is not customary for ingineering. The typical solution is to maximize the weighted function $W = \gamma_1 f_1 + \ldots + \gamma_n f_n$ where the weights $\gamma_k \geq 0$ are selected by the User. Changing the weights γ_k we could hope to investigate the multicriteria nature of the problem and to find a suitable compromise between inconsistent criteria.

Unfortunately, even if the optimization procedure is perfect the result could depend greatly on the selected weights unless the criteria $(f_1, \ldots, f_s)$ have their maxima at the same point $\vec{x}_+$. The straight line on the Fig. 1 (c) corresponds to the points with the same weighted value and the arrow shows its movement when the weighted sum is maximized over $\mathcal{F}$. It can be seen that with changing the inclination the abrupt jumps of the optimal point occur and that the part GH of the boundary is never checked by the weighted function. From the User's point of view it means that the method produces strange, unexpected and unstable results since even in simple cases a slight variation of the criteria weights could result to abrupt changes in position of the optimum point. (The weighted function works correctly only if $\mathcal{F}$ is a convex set; otherwise the abrupt jumps and high sensitivity to small variations of the weights and the model parameters are inavoidable.)

3 THE MAIN IDEA OF THE ALGORITHM *MULTI-BARS*

In practice in many cases the individual criteria functions cannot be differentiated and are strongly oscillating. Except the fact that the output of the Pareto set optimization is the ***continuous*** set of points, the Pareto set itself for the sets $\mathcal{F}$ with high dimension and complex topology can be very complicated. As a result all theoretical advantages of the Pareto set approach are of no use if there is no practical algorithm how to construct and how to work with Pareto sets.

To solve this problem the Pareto set the Multicriteria Branch Adaptive Random Search Method (*MultiBARS*) is proposed. Its predecessor the *BARS* method [2] was developed for single-criteria optimization with nondifferentiable criteria functions [3] and proved its reliability and stability.

The most simple way to demonstrate the base idea of *MultiBARS* is to show how to generalize the *Pure Random Search* (PRS) optimization for Pareto set approach. The PRS algorithm assumes that the random points are selected inside the set under consideration, and that the point with maximal (minimal) value of the merit function is accepted as the solution of the optimization problem. Although being very slow and unpractical, the PRS has a guaranteed convergence "with probability 1" to real optimum if some simple requirements are satisfied [4] (i.e., sample random points are distributed without gaps and holes inside the investigated set, and the optimum is not infinitely sharp).

The algorithm *Multi-PRS* algorithm can be constructed as follows. Suppose that $\mathcal{P}$ is the set of points selected as the discrete representatives of the Pareto set (at the beginning of the algorithm it is empty), $\vec{x} = (x_1, \ldots, x_n) \in \mathcal{X} \subset R^n$ is the random sample selected at some step, $\vec{p}$ in $\mathcal{P}$ is the element from $\mathcal{P}$, $\vec{f}_x = \vec{F}(\vec{x})$ is the criteria vector for $\vec{x}$, and $\vec{f}_p = \vec{F}(\vec{p})$ is the criteria vector for $\vec{p}$. The comparison of the criteria vectors is organized as follows:

- $\vec{f}_p \leq \vec{f}_x$ if all components of $\vec{f}_p$ are no greater than corresponding components of $\vec{f}_x$;
- $\vec{f}_p \geq \vec{f}_x$ if all components of $\vec{f}_p$ are no less than corresponding components of $\vec{f}_x$;

- $\vec{f}_p <> \vec{f}_x$ if some components of $\vec{f}_p$ are greater and some components of $\vec{f}_p$ are less than corresponding components of $\vec{f}_x$;
- finally, $\vec{f}_p = \vec{f}_x$ if all components of $\vec{f}_p$ are equal to corresponding components of $\vec{f}_x$.

Random sample vectoprs $\vec{X}$ are selected in $\mathcal{X}$ and tested:

- if there is such $\vec{p}$ in $\mathcal{P}$ that $\vec{f}_p < \vec{f}_x$, vector $\vec{p}$ is deleted from $\mathcal{P}$;
- if there is such $\vec{p}$ in $\mathcal{P}$ that $\vec{f}_p > \vec{f}_x$, sample vector $\vec{x}$ is discarded;
- if for all $\vec{p}$ in $\mathcal{P}$ $\vec{f}_p <> \vec{f}_x$, sample vector $\vec{x}$ is added to $\mathcal{P}$.

It can be shown easily that under some simple assumptions the set $\mathcal{P}$ converges "with probability 1" to the Pareto set although this convergence is very slow. *Multi-BARS* is constructed from *BARS* following the same idea although this algorithm is quite not so simple and trivial. The size of this publication does not enable to describe *Multi-BARS* in details, but the following features are essential:

- decomposition of the set $\mathcal{X}$ into *intensive search domain* ISD and the rest region $\mathcal{X} \setminus ISD$;
- adaptation of the ISD position and size depending on the results of the search;
- adaptation of the probability to search inside ISD and outside ISD;
- parallel search using several independent branches;
- cancelling and restarting the branches if two braches are too close to each other (i.e., if actually both branches perform the search in the same region);
- discarding some vectors from $\mathcal{P}$ when there is no memory to keep *all* generated vectors $\vec{p}$.

Numerical experiments show that *Multi-BARS* works well with nondifferentiable functions and non-convex sets and in most cases really enables to construct the discrete set of dense points which approximate the Pareto set.

4 EXAMPLES

The advantages of multicriteria approach is demonstrated using the optimization of the magnet mass-analysers of Mattauch-Herzog [5] and Cross [6] as an example (in Charged Particle Optics [7] these schemes are known for a long time and are widely used even in modern mass-spectrometers). The details and the discussion of the results represented here as the examples are briefly reviewed in [8].

Fig. 1 (a) shows the value of resolution R_s as the function of the parameter Ω near the canonical solution [5] usually cited in literature (here Ω is the toroidal factor of magnetic field). Other parameters considered below are fixed on this plot. We can see the strong sensitivity of the goal function to variations of this parameter.

Fig. 2 (b) shows the solution of the optimization of the same device with the criteria vector selected as $\vec{F} = \langle R_s, \Omega \rangle$, $R_s \to \max$, $\Omega \to \min$. Instead of strong oscillation of the function R_s many alternative variants appeare. The canonical scheme [5] is marked as a bulky black dot. The set of parameters is defined as $X = \{l'_c, r_c, \epsilon', l''_m\}$ where l'_c and r_c — the entry distance and radius of the electrostatic cascade, ϵ' and l''_m — entry angle and exit distance of the magnetic cascade.

Fig. 3 (c) shows the solution of the optimization problem $\vec{F} = \langle R_s, \Psi \rangle \longrightarrow \max_X$ for the Cross isotopic mass-spectrometer [6] (where R_s is the resolution and Ψ is the inclination angle of the focal line). The canonical scheme is marked as a bulky black dot too. Case A relates to 2 free parameters (entry and exit curvatures of the magnet boundaries), and case B adds entry and exit drift lengths and the rotation angle to this list. This example shows how the multicriteria approach gives the possibility to improve one criterion almost without get worse of another one.

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ANALYSIS OF THE UNCERTAINTIES IN THE IPCC DEFAULT METHOD FOR ESTIMATING N_2O EMISSIONS FROM AGRICULTURAL SOILS

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ABSTRACT

In this paper a quantitative uncertainty analysis of the methodology for estimating N_2O emissions from agricultural soils included in the IPCC Guidelines for National Greenhouse Gas Inventories is presented. For that purpose we applied the IPCC method to the Netherlands and analysed the results using Monte Carlo sampling techniques. The results indicate that the Dutch N_2O emissions from agricultural soils are 26 (15-44) Gg N in 1990. This range reflects a 95% confidence interval and is smaller than a range based on high and low parameter values only (5-60 g N/yr.). The results moreover indicate that four of the 16 parameters analysed have a relatively large impact on the overall uncertainty: the emissions factor for direct soil emissions (EF_1), the fraction of nitrogen input to soils that is lost through leaching and runoff ($Frac_{leach}$), the emission factor used to express leaching and runoff leading to indirect emissions (EF_5) and the total nitrogen excretion by animals in the country (Nex).

1 INTRODUCTION

Monitoring anthropogenic emissions of pollutants to the atmosphere is an area of rapidly growing interest both in the scientific community and in policy making. Several methodologies to estimate emissions have been developed. These methods, however, seldom take into account the uncertainties in the estimates. According to Gardner et al. (1988) [1], the usefulness of any given model depends on the accuracy and reliability of the model prediction. In the case of emission inventories the knowledge and information on the processes involved is usually limited and uncertain. In order to asses the accuracy and reliability of a model, an analysis of the uncertain aspects is needed. Usually emission estimates are established by direct monitoring at each emission source or by using activity data and emission factors [2] [3]. Both methods will result in an estimate of the 'real' emission. The difference between the estimated emission and the real emission is the uncertainty of the emission inventory. Uncertainties in the emission estimate can be assessed by comparing the emission estimate to a direct measurement. Emission measurements, however are not always available. Alternatively, comparison of models can give qualitative information on the most uncertain aspects of the inventory. If comparable models are also not available, statistical analysis can be a applied to determine which model parameters have large influence on the model output (sensitivity). Combining the information on sensitivity with information on possible values of key parameters can give an estimate of the model uncertainty. In this study we want to consider the usefulness of sensitivity and uncertainty analysis of an emission model which is regarded as relatively uncertain and for which very few measurements and no comparable models are present at this moment. Therefore, here the uncertainty in an emission methodology for N_2O emissions from agricultural soils is analysed by performing an uncertainty analysis.

2 METHOD FOR ESTIMATING N_2O FROM AGRICULTURAL SOILS ACCORDING TO IPCC GUIDELINES

Nitrous oxide (N_2O) is a greenhouse gas. Sources of N_2O are agriculture, natural processes, fossil fuel combustion, waste treatment and industry. The IPCC Guidelines for National Greenhouse Gas Inventories (hereafter referred to as IPCC method) provide default methodologies for estimating anthropogenic greenhouse gas emissions on a national scale. Here we will investigate uncertainties in the IPCC method for estimating emissions of nitrous oxide from agricultural soils (box 1; for a detailed description is referred to IPCC/OECD (1997) and Mosier et al. (in press) [4] [5]). The IPCC method is analysed with the Netherlands as country of study.

Table 1 Values and distribution of parameters in the IPCC method [4,3] for the Netherlands (1990).

Name	Explanation	Unit	Distribution	Mean	Variance	Minimum	Maximum
$Crop_{bf}$	dry pulses and soybeans produced	kg/yr	constant[3]	83 E+6[5]	-	-	-
$Crop_0$	dry production of other crops	kg/yr	constant[3]	1352 E+6[5]	-	-	-
F_{os}	area of cultivated organic soils (	ha	constant[3]	274124[6]	-	-	-
N_{fert}	use of synthetic feriliser	kg N/yr	constant[3]	412 E+6	-	-	-
$Frac_{graz}$	fraction of livestock nitrogen contained in excrements deposited during grazing	kg N/kg N	constant[3]	0.13[4]	-	-	-
Nex	total nitrogen excretion by animals	kg N/yr	triangular[8]	780 E+6[4]	-	567 E+6[8]	1043 E+6[8]
Nex_{prp}	nitrogen excretion by animal waste management system	kg N/yr	triangular[8]	103 E+6[4]	-	52 E+6[8]	203 E+6[8]
Yield	yield of nitrogen fixing crops	-	triangular[8]	2[3]	-	1.5[8]	2.5[8]
$Frac_{burn}$	fraction of crop residue that is burned	kg N/kg N	triangular[8]	0.0[3]	-	0.0[8]	0.1[8]
$Frac_{fuel}$	fraction of livestock nitrogen excretion contained in excrements burned for fuel	kg N/kg N	triangular[8]	0.0[3]	-	0.0[8]	0.3[8]
$Frac_{gasf}$	fraction of total synthetic fertiliser that is emitted as NO_x + NH_3	kg NH_3-,N NO_x-N/kg fertiliser	triangular[8]	0.1[3]	-	0.01[8]	0.2[8]
$Frac_{gasm}$	fraction of total nitrogen excretion that is emitted as NO_x and NH_3	kg NH_3-N, NO_x-N/kg synthetic fertiliser	triangular[8]	0.2[3]	-	0.01[8]	0.3[8]
$Frac_{leach}$	fraction of nitrogen input to soils that is lost through leaching and runoff	kg N/kg fertiliser,manure	triangular[8]	0.3[3]	-	0.1[8]	0.5[8]
$Frac_{ncbf}$	fraction of nitrogen in N-fixing crops	kg N/kg dry biomass	triangular[8]	0.03[3]	-	0.02[8]	0.04[8]
$Frac_{ncr0}$	fraction of nitrogen in not-N-fixing crops	kg N/kg dry biomass	triangular[8]	0.015[3]	-	0.005[8]	0.025[8]
$Frac_r$	fraction of crop residue that is removed from the field as crop	kg N/kg crop-N	triangular[8]	0.45[3]	-	0.3[8]	0.7[8]
EF_2	emission factor for organic soil mineralisation due to cultivation	kg N/ha,yr	triangular[8]	5[3]	-	2[8]	15[8]
EF_1	emission factor for direct soil emission	kg N_2O-N/kg nitrogen input	normal[1]	0.0125[1]	0.0000178[1]	0.00402[1]	0.0209[1]
EF_3	emission factor for animal waste management system	kg of Nex in AWMS	normal[2]	0.02[2]	0.0000284[2]	0.005[2]	0.03[2]
EF_4	emission factor for atmospheric deposition	kg N_2O-N/kg NH_3-N, NO_x-N emitted	normal[2]	0.01[2]	0.0000142[2]	0.00321[2]	0.0165[2]
EF_5	emission factor for leaching runoff	kg N_2O-N/kg leaching	normal[2]	0.025[2]	0.0000356[2]	0.00803[2]	0.0414[2]

1. based on Bouwman, 1995, 2. Scaled to Bouwman, 1995, 3. IPCC,1997, 4. Bogdanov & Kroeze, in press, 5. FAO, 1990, 6. Kroeze, 1994, 7. RIVM, 1993, 8. expert judgement/educated guess

Box 1: Nine equations summerizing the IPCC default method for estimating N_2O emissions from agricultural soils. See table 1 for explanation of variable names.

Equations:

(1) $F_{sn} = N_{fert} \times (1\text{-}Frac_{gasf})$

(2) $F_{aw} = (Nex \ (1\text{-}Frac_{fuel} + Frac_{graz} + Frac_{gasm})$

(3) $F_{bn} = Yield \times Crop_{bf} + Frac_{ncbef}$

(4) $F_{cr} = Yield \times [\ Crop_0 \times Frac_{ncr0} + Crop_{bf} \times Frac_{ncrbf}] \times (1\text{-}\ Frac_r) \times (1\text{-}Frac_{burn})$

(5) $N_2O_{animals} = N_2O_{prp} = Nex_{prp} \times EF_3$

(6) $N_2O_{direct} = [F_{sn} + F_{aw} + F_{cr} + F_{bn}] \times EF_1 + F_{os} \times EF_2$

(7) $N_2O_{(g)} = (N_{fert}) \times Frac_{gasf} - Nex \times Frac_{gasm}) \times EF_4$

(8) $N_2O_{(l)} = (N_{fert} + Nex) \times Frac_{leach} \times EF_5$

(9) $N_2O = N_2O_{direct} + N_2O_{animals} + N_2O_{(g)} + N_2O_{(l)}$

The IPCC method distinguishes between three types of N_2O emissions from agricultural soils (i) direct emissions from agricultural fields, induced by N-inputs, (ii) direct soil emission following manure production by grazing animals, and (iii) indirect emissions, taking place after the nitrogen leaves the field. The related N_2O emissions are calculated in nine steps (box 1). Default parameters are shown in Table 1.

3 UNCERTAINTY ANALYSIS

The basis of the sensitivity and uncertainty analysis performed here is Monte Carlo Sampling. We used the UNCSAM (**unc**ertainty analysis by Monte Carlo **sam**pling techniques) software package [6] . The sampling technique applied in our analysis is Latin Hypercube Sampling (LHS) which uses a stratified way of sampling from the separate parameters. Applying LHS sampling techniques requires that the number of samples is 4/3 * number of parameters (p) with a minimum of 2p and a maximum of 5p [6] . We included 16 of the 21 parameters that are distinguished in the IPCC method in our analysis by 100 samples. In order to implement the IPCC method for the Dutch situation in UNCSAM the values, distribution and possible correlation of the parameters are defined as show in Table 1. Parameter values are default values from IPCC/OECD (1997) [5] unless mentioned otherwise (Table 1). The distributions of the non-constant parameters were based on expert opinion,except for EF_1, EF_3, EF_4 and EF_5.

4 RESULTS AND CONCLUSIONS

(i) Total uncertainty of the model output

Total uncertainty of the resulting model outputs can be expressed by presenting for instance the frequency distribution, basic statistics and the confidence bounds of the cumulative distribution. Figure 1 presents the distribution of the calculated Dutch emissions and Figure 2 the 95% confidence interval for the cumulative distribution.

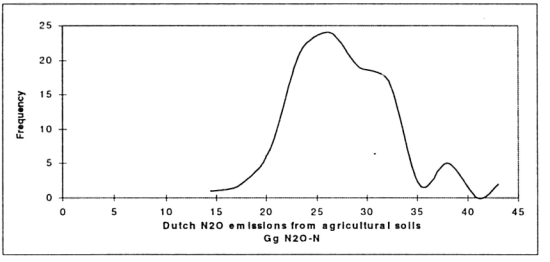

Figure 1. Frequency distribution of Dutch (1990) N_2O emissions from agricultural soils, calculated following the IPCC guidelines [4,5] while using Latin Hypercube sampling for choosing parameter values (100 samples).

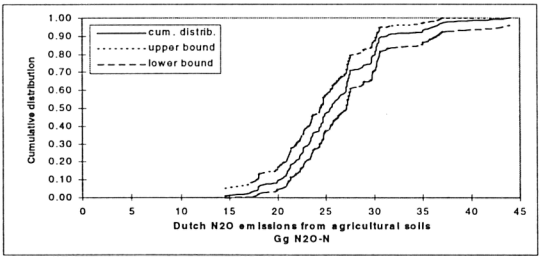

Figure 2. 95% confidence interval for the cumulative distribution of Dutch (1990) N_2O emissions from agricultural soils, calculated following the IPCC guidelines [4,5] while using Latin Hypercube sampling for choosing parameter values (100 samples).

The Dutch N_2O emission is calculated to be 26.1 Gg N/year as mean with an absolute uncertainty of 5.27 Gg N/year which is 20% of the mean value. The skewness shows that the distribution is extending towards more higher values, with a minimum of 14.5 Gg N/year and a maximum of 44.0 Gg N/year (Fig. 1). This range is much smaller than the theoretical range of 5 to 60 Gg N based on high and low parameter values.

(ii) Uncertainty contribution of the individual parameters.

Since the IPCC method is a linear model without correlation between the individual parameters, the sensitivity and contribution to total uncertainty can be expressed by one measure[6]. As measure for the sensitivity and uncertainty we chose the standard regression coefficient (SRC). SRC measures the relative change (Δy) of model output (y) in terms of its standard deviation (S_y), if parameter (x) changes relatively in terms of its standard deviation S_x, while the other parameters remain constant. The linear regression resulted in an R^2 of 0.985 indicating that the linear regression model accounts for 98.5% of the total uncertainty. The results indicate that the IPCC method is sensitive for values of the parameters EF_1, $Frac_{leach}$, EF_5 and Nex and that the total uncertainty of 20% is largely caused by these parameters with EF_1 as the largest source of uncertainty (see table 1 for explanation of variable names). EF_1 is the emission factor used for calculating the direct soil emission of N_2O and based on all measurements (Bouwman,1995)[7]. The second most important contributors tot total uncertainty are $Frac_{leach}$ and EF_5. $Frac_{leach}$ expresses the fraction of nitrogen input to soils that is lost through leaching and runoff. This parameter is based on expert opinion (IPCC/OECD, 1997) [5]. EF_5 is an emission factor used to express leaching/runoff leading to indirect emissions and is determined by expert opinion and based on EF_1. Another large contributor is Nex which expresses the total nitrogen excretion by animals in the country (Bogdanov and Kroeze, 1996) [8]. This study showed that sensitivity and uncertainty analysis can be a useful tool in analyzing the uncertainties in the IPCC method. It may help in improving the quality of emission inventories.

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SENSITIVITY ANALYSIS OF A MULTILEVEL MODEL: NOTION AND SOME EXAMPLES

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1 INTRODUCTION

"Sensitivity analysis yields the changes of the model output in response to systematic changes in the output" [1]. Using an more or less complicated input-output model an analysts make a change in the input of the model and they see what changes in the output. In order to do this type of anlysis it is necessary that the model is carefully specified, especially that the type of units are clear. However, the specification and identification of the type of units seems to be to have received minor attention. However, although [1] distinguishes the environmental type and control type of input variables, he did not draw from it the consequence that in the case of control variables take the form of policy measures, it mostly means the conditioning or steering of lower level processes by a higher level. [2] further advocates that sensitivity analysis is most relevant for environmental variables. However, the outcomes of a sensitivity analysis, in their turn, can be viewed as outputs which are sensitive to control variables as an input.

Thus, it is worthwhile to split the environmental variables of a lower level from the control variables on a higher level as two independent sources of variance. As a result, there are two independent sources of sensitivity according to both levels. Although the sources themselves are independent, they are mutually ordered in a very special manner. They are ordered according to a nested structure. The processes that originate from the environmental input variables which belong to the same unit as the output variables, to be described as a black box or not, are on the lower level. Mostly this level concerns individuals, but it can also concern groups or divisions of organizations. The processes which originate from control variables and other variables which concern meaningful aggregates of lower level units are on the higher level. Mostly it concern groups, organizations or even countries. This implies that the inputs of a lower level unit within a same higher level unit are *more alike* than the input between the higher level units. It is obvious, that this very assumption has to underly the model of analysis.

The multilevel regression metamodel of analysis is appropriate to this. It enables to decompose both types of variance mentioned and to detect the level-specific contributions to each type of variance. In such a multilevel design it is typically assumed that the units of the various levels are obtained by multiple sampling: the higher level units are randomly sampled from a population of higher level units, and thereafter, *within* each higher level unit, the lower level units are randomly sampled from a population of higher level units.

The aim of this paper is asking attention for the multilevel sensitivity analysis and the corresponding multilevel regression metamodel. Two illustrations will be added. One illustration concerns the question of how to organize schools appropriate for offering students the best chances for good tracks. It implies a sensitivity analysis for a number of student inputs on the lower level and a sensitivity analysis of some school characteristics on the higher level. The second illustration concerns the question how eldery people's minor depression depends on time and how these 'depression trajectories' depend on stable and varying individual characteristics. It involves a sensitivity analysis of time and varying individual characteristics on the lower level and an analysis into the sensitivity of constant individual inputs.

2 THE MULTILEVEL MODEL

The random coefficient regression model of multilevel analysis can be defined as an approximative metamodel for input-output analysis. In the first part of this section we describe a general model, and in the second part a model that is especially derected to describe developments in time.

2.1 General model

The multilevel model can be described fundamentally as constisting of two equations [3, 4, 5]. The first equation (regarding level 1) concerns the within-group regression where an output variable is explained by a number of input variables. The erroneously neglected input variables, measurement errors and estimation errors are expressed in the disturbance term (e_{ij}). With respect to lowel level unit i and the higher level unit j the equation is as follows:

$$Y_{ij} = \beta_{0j} + \beta_{1j} X_{1ij} + \beta_{2j} X_{2ij} + \ldots + \beta_{kj} X_{kij} + e_{ij} \quad (1)$$

where i: the lower level unit (i= 1,...,I), j: the higher level unit (j = 1,...,J), Y_{ij}: output variable, X_{ki}: input variables (k = 1,...,k) for i, β_{0j}: the intercept for j, β_{kj}: the regression coefficient of the output variable Y_{ij} on the input X_{ki}, and e_{ij}: the disturbance term belonging to Y_{ij}, with variance σ^2 and mean 0. The second equation on the level of the higher level units specifies the regression of the lower level coefficients β_{kj} (k = 0, 1,...,K) on the higher level characteristics incorporated. As a result, a new regression equation is formulated for each coefficient. It is formulated as follows:

$$\beta_{kj} = \gamma_{k0} + \gamma_{k1} Z_{1j} + \ldots + \gamma_{kN} Z_{Nj} + u_{kj} \quad (2)$$

where Z_{nj}: higher level input variables (n = 1,...,N) for j, γ_{k0}: the intercept of the regression, γ_{kn}: the regression coefficient of the output variable β_{kj} on the input higher level variable Z_{nj}, and u_{kj}: The disturbance term belonging to β_{kj}, with variance σ^2_k and mean 0. The common assumptions are valid; moreover it is supposed that $\rho(z,e) = 0$.

By substituting equation (2) into equation (1) we get the final model for i. It expresses the differences of the input-output processes on the higher level, expressed by σ^2_k, if the higher level variables are absent. If any σ^2_k is not equal to zero, it is worthwhile to introduce the higher level variables into the analysis.

On the basis of this structure of units the variance of a given variable can be decomposed according to each level, and the resulting types of variance can be regressed on a set of input variables on the lower level unit. There is also a covariance matrix of the disturbances on the higher level. It seems that this is in line with [6, 7].

2.2 Developments in Time.

If the sensitivity analysis is done using the multilevel variant of the regression metamodel of analysis, the main input variable is time. Hence, here we use especially the longitudinal multilevel model (See also [8, 9]). The model basically consists of two equations. In the first equation, which relates to the occasions of measurement (level-1), a given output is regressed on the time-axis (in principle according to a polynomial function). The simplest corresponding equation is the following one.

$$Y_{ij} = \beta_{0j} + \beta_{1j} t_{ij} + e_{ij} \quad (3)$$

where Y_{ij} is the output variable. The symbol t expresses the time variable. This expression corresponds to the equation of the regression of Y on t, but it is somewhat more complicated than that. The complication appears in the subscripts. i refers to occasions (i = 1,...,I,) and j to individuals (j = 1,...,J). The subscripts i and j attribute the score to both sources of variance, being the occasion and the individual respectively. The intercept, being a constant for all occasions per individual, is expressed by β_{0j} and the regression slope is indicated by β_{1j}. Said more specifically, β_{1j} indicates the multiplication factor for predicting a change in Y on the base of a change of one point on the scale of t. The subscript j refers to the variability of the intercepts and the slopes across the individuals. e_{ij} expresses the disturbance term belonging to Y_{ij}; $E(e_{ij}) = 0$; $Var(e_{ij}) = \sigma^2_e$. This term e_{ij} indicates the deviation of a score of Y_{ij} in a given occasion from the prediction from $\beta_{0j} + \beta_{1j} t_{ij}$ for respondent j. In short, equation (1) describes the developmental functions of Y of individuals in time.

Next, the inter-individual comparison has to be introduced into the model. For simplicity's sake, let we start again from equation (3). For each individual the intercept β_{0j} can be decomposed into a mean value γ_0, which is common to all individuals, and a specific deviation u_{0j}. Moreover, for all individuals the slope β_{1j} can be decomposed in a common, mean slope γ_1 and a specific deviation u_{1j}.

$$\beta_{0j} = \gamma_0 + u_{0j} \quad (4a)$$
$$\beta_{1j} = \gamma_1 + u_{1j} \quad (4b)$$

- This offers:

$$Y_{ij} = \gamma_0 + \gamma_1 t + u_{0j} + u_{1j} t + e_{ij} \quad (5)$$

Equation (5) shows that the scores on Y of an individual j in a given occasion i are expressed in terms of t, the individual-related deviations u_{0j} and u_{1j}, and the occasion-bound deviation e_{ij}. The variance of u_{0j} is indicated by σ^2_{u0}, the variance of u_{1j} by σ^2_{u1}. Their covariance is expressed by σ^2_{u0}. Those coefficients refer to the variances and covariance of the intercept parameters β_{0j} and slope parameters β_{1j}. It is assumed that there is no correlation between

the occasion disturbance term and the both individual disturbance terms: $E(u_{0j}) = E(u_{1j}) = Cov(u_{0j},e_{ij}) = Cov(u_{1j},e_{ij}) = 0$.

Now the interrelation of the inputs measured at a same occasion. These concern individual variables that vary over time. The interrelation can be described by extending equation (5) by such a variable, say X_{ij}. The subscript i indicates the simultaneous measurement of X_{ij} as Y_{ij}. As a corresponding slope coefficient α_{ij} is introduced. This gives a formula for analysizing sensitivity of an output variable on both time and time-varying individual input variables.

$$Y_{ij} = \beta_{0j} + \beta 1 t_{ij} + \alpha_i X_{ij} + e_{ij} \tag{6}$$

The question now can rise about the explanation of the interindividual relations among differences in developmental courses by individual variables. This question give rise in extending the last equation. Again for simplicity's sake, using the regression model of analysis we restrict ourselves to only one individual input variable.

For intercepts it yields

$$\beta_{0j} = \gamma_{00} + \gamma_{01} Z_{1j} + u_{0j} \tag{7a}$$

and for slopes

$$\beta_{1j} = \gamma_{10} + \gamma_{11} Z_{1j} + u_{1j} \tag{7b}$$

Here, it is investigated whether the variances of the intercept parameters β_{0j} and slope parameters β_{1j} are reduced by the individual *constant* variable Z_{1j}, say education. This analysis gives rise to answering questions like "Is an individual output variable sensitive on their level of education?" (regarding the intercept), and "Is the change in individuals' depression level over time sensitive to their level of education?" (regarding the slope). In the example, it is supposed that a person's level of completed education is a constant.

In an analogous way questions about sensitivities of relations of an dependent variable and *varying* input variables W to be found in individual constant variables can be answered. An example is: "Is the strength of the relation of, say, perception of physical health on depression at the time occasion sensitive to level of education?", where somebody's perception of physical health can vary in time. The corresponding simplified formula sounds as follows:

$$\alpha_{0j} = \gamma_{00} + \gamma_{01} W_{1j} + u_{1j} \tag{8a}$$

$$\alpha_{1j} = \gamma_{10} + \gamma_{11} W_{1j} + u_{1j} \tag{8b}$$

Now we are able to formulate more generally the second basic equation of the multilevel longitudinal model. The second equation is on the respondent level (level-2) and describes how the regression of the β_{0j}-coefficients of the first equation on the time-descriptors depend on respondent variables. This occurs by incorporating relevant individual covariates Z_{nj} with respect to Y_{ij} into the equation by adding the term $\gamma_{n1}Z_{1j} + ... + \gamma_{nS}Z_{Sj}$ for each β_{nj} in the right part of the equation, taking with it the intercept γ_{n0} and the disturbance term u_{nj}. They explain occurring individual differences in the functions. As a result, the following regression equation is formulated for each coefficient:

$$\beta_{0j} = \gamma_{00}Z_{0j} + \gamma_{01}Z_{1j} + ... + \gamma_{0S}Z_{Sj} + u_{0j} \tag{9a}$$

and

$$\beta_{1j} = \gamma_{10}Z_{0j} + \gamma_{11}Z_{1j} + ... + \gamma_{1S}Z_{Sj} + u_{1j} \tag{9b}$$

where: Z_{nj} refers to the input variables ($n = 0,1,...,N$) for individual j, γ_{nn} is the regression coefficient of the individual 'output variable' β_{nj} on the individual input variable Z_{nj}; $Z_{0j} = 1$. u_{nj} indicates the disturbance term belonging to β_{nj} assuming that $E(u_{nj}) = 0$; $Var(u_{nj}) = \sigma^2_{nn}$; $Cov(u_{nj},u_{ij}) = \sigma_{nn'}$; $Cov(e_{ij},u_{nj}) = 0$. The common assumptions with respect to regression analysis yield; moreover it is supposed that $Cov(e,u) = 0$. If we delete Z_{nj} out of the equation, the disturbances equal to:

$$u_{0j} + u_{1j}t_{ij} + u_{2j}t_{ij}^2 + ... + u_{Rj}t_{Rij}^R + e_{ij} \tag{10}$$

offering the random part of the model:

$$\sigma_0^2 + 2t_{ij}\sigma_{01} + t_{ij}^2\sigma_1^2 + \ldots + t^2\sigma_R^2 + \sigma_e^2 \qquad (11)$$

the variance of each term of

$$\sigma_0^2 + (t_{ij} + t_{i'j})\sigma_{01} + t_{ij}t_{i'j} + \ldots + t_{ij}t_{i'j}\sigma^2 \qquad (12)$$

The fixed part of the model is constituted by the model without the random part.

As known, the ratio of the level-2 variance (σ_{u0}^2) to the total variance ($\sigma_{u0}^2 + \sigma_e^2$) is called the 'intra-unit correlation' or 'clustering effect', ρ. Since on level-1 t_{ij}^r-variables and on level-2 Z_{uj}-variables are incorporated in the equation, their variances have been corrected, resulting in a corrected intra-unit correlation, ρ_{corr}.

Since equations are very simple, a more general equation is needed. It takes the form of

$$Y_{ij} = \beta_0 + \beta_1 t_{1ij}^1 + \beta_2 t_{2ij}^2 + \ldots + \beta_R t_{Rij}^R + \alpha_1 X_{1ij1} + \alpha_2 X_{2ij1} + \ldots + \alpha_N X_{Nij1} + e_{ij} \qquad (13)$$

where t_{ij}^k the fixed time variable ($k = 0, 1,\ldots,K$) for individual j, and r the power of the polynomial function ($r = 0, 1,\ldots,R$). Since $t_{0ij}^0 = 1$, this term can be omitted. β_{ij} indicates the regression coefficient of the output variable Y_{ij} on t_{ij}^R and α_{nj} its regression coefficient on the time-varying input individual variable X_{nij} ($n = 0,\ldots,N$). β_{ij} is a general intercept. The common assumptions of regression analysis apply.

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SENSITIVITY ANALYSIS OF RELIABILITY-BASED OPTIMIZATION IN SEA DIKE DESIGNS

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ABSTRACT

The reliability concept is now widely accepted in civil engineering as a tool to find the most appropriate structural system in terms of safety and economy. Design engineers can determine the optimum degree of safety for a structure to satisfy the safety demands and economical concerns of owners or users. One of the difficulties however in applying a reliability-based optimization lies in the lack of supporting data that can be used in the associated probability-based decision models. Also the uncertainty in the economic parameters of structural systems can cause difficulties in the optimization procedures. In this paper a sensitivity analysis will be performed in the reliability-based optimization of a sea dike design in the Netherlands. The Netherlands is a low-lying country which has to protect itself against flooding from the sea and its rivers. Reliable flood defenses are essential for the safety of the country. In a sea dike design one has to take account for a lot of uncertainties. These uncertainties are caused on one hand by the lack of sufficient data of extreme water levels (leading to a frequency distribution with stochastic parameters) and on the other hand by the uncertainty in construction costs and failure costs. The influence of these uncertainties causes the reliability-based optimal dike height to rise quite substantially.

1 INTRODUCTION

Probabilistic design of flood protection has become quite accepted nowadays. Already in the late 1950's a very extensive research project was initiated in the Netherlands by the Delta Committee on the probabilistic analyses of flood defences [1,2]. Since then many research projects on the field of risk-based decision-making in flood protection followed of which [3,4] give good overviews. In the design of dikes, many uncertainties play an important role. However, the influence of uncertainties in for example construction costs, damage costs and statistical uncertainty hasn't been investigated in a probabilistic framework so far. Statistical uncertainty due to a limited amount of data can be approached very well by Bayesian statistics. Van Gelder [5] showed how to deal with statistical uncertainty for sea level data along the Dutch coast. In this paper we will discuss the reliability-based optimal model for dike design in section 2. In sections 3 and 4 the statistical-, construction- and damage uncertainty on the economical dike design will be investigated.

2 RELIABILITY-BASED OPTIMAL MODEL

In this section the economic-mathematical model of Van Dantzig [1] will be discussed for the construction of dikes. Assume that an existing dike has a height of H_0. The dike will be heightened to an optimal height H. The costs involved with this heightening are a function of X where $X = H - H_0$. These costs can be assumed linearly with X by the relation:

$I = I_0 + I'X$ in which:
I_0 are the mobilisation costs and
I' are the costs per meter dike heightening.

In Van Dantzig's model, the only failure mechanism of dikes that is considered is overtopping. If the waterlevel h is higher than the dike height H, then inundation takes place with a total damage of W. The probability of inundation can be modeled in many different ways and is still a very controversial subject [6]. Van Dantzig choose the exponential distribution function for modeling the probability of inundation at Dutch coast near Hook of Holland:

$$F(h)=1-e^{-(h-A)/B} \quad (h>A) \tag{1}$$

The expectation of the damage per year is now given by F(h)W and the expectation of damage over the lifetime of the dike is $\bullet \int F(h)W/(1+r)^i$ with $i = 1..\infty$, which can be simplified to F(h)W/r with r the discount factor.

The total costs are therefore given by the expression:

$$K(X) = I + R = I_0 + I' X + \frac{W \cdot F(H_0 + X)}{r},$$

which is the summation of construction costs and discounted damage expectation. The optimal dike heightening X_{opt} can be found by solving the equation $dK(X)/dX = 0$.

3 SENSITIVITY ANALYSIS OF THE STATISTICAL UNCERTAINTY

The probability of inundation is determined on a dataset of annual maxima of water levels at the location of Hook of Holland from the period of 1887 till 1996. In [5], it is described how model and statistical uncertainties can be determined with Bayesian methods and it is applied on the Hook of Holland dike. The results are summarized in the next table:

Table 1: Influence of statistical and model uncertainties on the reliability-based optimal dike height

	Opt. dike height[m]	Prob. of inundation	Costs [gld]	Opt. dike height[m]	Prob. of inundation	Costs [gld]
	Exponential Model			Gumbel Model		
Without stat. Uncertainty	5.88	7.52×10^{-6}	157×10^{6}	5.51	6.43×10^{-6}	141×10^{6}
With stat. Uncertainty	6.00	8.38×10^{-6}	164×10^{6}	5.67	7.24×10^{-6}	148×10^{6}

We observe a higher optimal dike height if we include statistical uncertainty in the economic optimization procedure both for the exponential and the Gumbel model. Consequently also the probabilities of inundation increase as well as the total costs increase as uncertainty is taken into account.

4 SENSITIVITY ANALYSIS OF CONSTRUCTION COSTS AND DAMAGE COSTS UNCERTAINTY

Apart from statistical uncertainty there is also uncertainty in the costs of dike heightening (i.e. the parameters I_0 and I'), and in the damage costs W. In this section the influence of the uncertainty in the parameters I_0, I' and W will be analyzed. We consider these parameters as random variables with a normal distribution. Formula (2) becomes:

$$\underline{K}(X) = \underline{I} + \underline{R} = \underline{I_0} + \underline{I}' X + \frac{p \underline{W}}{r} \qquad (3)$$

Rather than optimizing $\mu(K)$, as is done in the Van Dantzig calculation, we will optimize $\mu(K)+k\sigma(K)$, in which k is the risk aversion index [7]. Risk averse designers will tend to chose a high k (k towards 2) and invest more in a design to be sure of a safe structure. The influence of the uncertainty in the cost - and damage variables and the choice of the risk aversion index on the optimal dike height will be analyzed next. Costs of dike heightening can be quite well estimated on before hand. Therefore we assign to I_0 and I' a variation coefficient of 10%. Costs of damage caused by inundation is more difficult to estimate, leading to a variation coefficient for W of 30%.

In figure 1, we have plotted the mean cost function added with k times the standard deviation of the costs (k=0,½,1 and 1½). In table 2, the results of the optimal dike height are shown. We observe that a higher risk aversion leads to a higher optimal dike height, which gives a safer construction (the probability of inundation decreases), but at the same time higher construction costs. For example if we add one standard deviation in the optimization procedure, the total costs increase 50% but the safety increases 2000%.

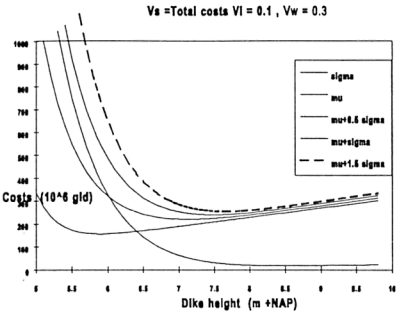

Figure 1: • (K)+k• (K) for different values of k

Table 2: Results of optimization

Risk avers index	Minimal Costs, [10^6gld].	Opt. dike height [m]	Prob. of inundation
k=0	157	5,88	$7{,}52.10^{-6}$
k=½	221	7,13	$1{,}18.10^{-7}$
k=1	241	7,48	$3{,}70.10^{-7}$
k=1½	255	7,65	$2{,}10.10^{-8}$

The influence of the value of the variation coefficient has been investigated. It appears that V_W has a very low influence on the optimal dike height. The reason for this can be explained if we look at the variance of the total costs which contains a factor • ^{2}(W) + (1-p)• ^{2}(W). This can be approximated almost by the second term solely because • ^{2}(W)»• ^{2}(W). In the optimization procedure of • (K)+k• (K), there is therefore negligable influence of • (W). The influence of the variance of I' is however much larger. The higher the variation coefficient of I', the lower the optimal dike height, but the higher the total costs. From a coefficient of 10% to 50%, we observe an increase of about 20% in the total costs, and a decrease in optimal dike height of about 30cm.

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A SENSITIVITY ANALYSIS FOR INFORMATIVE DROPOUT: A LOCAL INFLUENCE APPROACH

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1 THE LINEAR MIXED MODEL

In medical research, studies are often designed in which specific parameters are measured repeatedly over time in the participating subjects. This allows to model the process of change within each subject separately, based on both subject-specific factors (such as age) and experiment-specific factors (such as treatment). The analysis of such *longitudinal data* requires statistical models which take into account the association between the measurements within subjects. During the last decade, a lot of effort has been put into the search for flexible longitudinal models. An overview can be found in Diggle, Liang and Zeger [3]. A frequently used model for continuous responses is the *linear mixed-effects model* (Laird and Ware [5], Verbeke and Molenberghs [10]) which assumes that, for each subject separately, the vector Y_i of repeated measurements satisfies the linear regression model

$$Y_i = X_i ff + Z_i b_i + "_i, \quad i = 1, \ldots, N$$

in which ff is a vector of population-averaged regression coefficients called fixed effects, and where b_i is a vector of subject-specific regression coefficients called random effects. Further, the b_i are assumed to be i.i.d. $N(0, D)$, and independent of the residual components $"_i$ which are assumed i.i.d. $N(0, \Sigma_i)$. Marginally, Y_i is then normally distributed with mean $X_i ff$ and covariance matrix $V_i = Z_i D Z_i' + \Sigma_i$, and all parameters in this marginal model can be estimated using standard techniques such as maximum or restricted maximum likelihood estimation.

2 THE PROBLEM OF DROPOUT

Note that the linear mixed model does not assume that an equal number of observations is available for all subjects. However, if unequal numbers of observations are the result of patients dropping out from the study, Rubin [8] has shown that valid inferences are obtained only when the missing data are *missing at random (MAR)*, i.e., when the non-response process does not depend on the unobserved outcomes. If this is not the case, the dropout is said to be *informative (ID)*. Diggle and Kenward [2] and Molenberghs, Kenward and Lesaffre [7] have shown that progress can be made by combining a model

for the *measurement process* (e.g. the linear mixed model) with a model for the *dropout process*, such as

$$\text{logit}\,[p_k(y_{i1}, y_{i2}, \ldots, y_{ik})] \;=\; \beta_0 \;+\; \beta_1\, y_{ik} \;+\; \sum_{j=2}^{k} \beta_j\, y_{i,k+1-j}, \quad i = 1, \ldots, N, \tag{1}$$

possibly extended with external covariates, some of which may vary with time. We hereby denote the jth observation for the ith subject by y_{ij}, and the dropout probability at time k by $p_k(\cdot)$. When β_1 equals zero, the dropout model is random, and all parameters can be estimated using standard software since the measurement model (a linear mixed model) and the dropout model (a logistic regression model) can then be fitted separately. If $\beta_1 \neq 0$, the dropout process is assumed to be informative. Rubin [9] points out that such analyses heavily depend on the assumed dropout process while it is impossible to find evidence for or against the model, unless supplemental information on the dropouts is available. Further, note that in practice, subjects may drop out for a variety of reasons, leading to some subjects dropping out at random while others drop out informatively. This is also not taken into account in the above model.

3 LOCAL INFLUENCE

In this paper, we investigate the *sensitivity* of the estimation of the quantities of interest (such as treatment effect or growth parameters) with respect to assumptions about the dropout model. Our dropout model under consideration is

$$\text{logit}\,[p_k(y_{i1}, y_{i2}, \ldots, y_{ik})] \;=\; \beta_0 \;+\; \omega_i\, y_{ik} \;+\; \sum_{j=2}^{k} \beta_j\, y_{i,k+1-j}, \quad i = 1, \ldots, N, \tag{2}$$

in which different subjects give different *weights* to the response at time k to predict dropout at time k. If all ω_i equal zero, the model reduces to a MAR model, hence (2) can be seen as an extension of the MAR model, which allows some individuals to drop out in a "more informative" way ($|\omega_i|$ large) than others ($|\omega_i|$ small).

Using the *local influence* approach of Cook [1], we study the sensitivity of the results obtained under the MAR assumption with respect to small perturbations of the ω_i around $\omega_i = 0$. For any N-dimensional unit vector l, a measure $C_{\mathbf{l}}$ of local influence can be calculated expressing local changes in the maximized likelihood function with respect to infinitesimal perturbations of the ω_i in the direction of l.

Several choices of l may be of specific interest, all leading to specific perturbations of the MAR model. One evident choice corresponds to the direction of the ith subject, i.e., the vector l contains zeroes everywhere except on the ith position where there is a one. The so-obtained influence measure C_i expresses how the MAR results change (locally) when the model is extended in the direction of informative dropout for the ith subject. A large value for C_i suggests that the dropout probability of subject i at time k may not only depend on that subject's history up to time k but also on its response value y_{ik} at time k, and therefore that the informative dropout model may be appropriate for this subject. On the other hand, a small value for C_i suggests that the dropout probability of subject i at time k only depends on that subject's history up to time k, and therefore that the MAR assumption is appropriate. As shown by Lesaffre and Verbeke [6] in another context, the analytic expressions for the C_i allow to decompose the C_i into interpretable components. This yields additional insights in the reasons why some subjects are more influential than others. This is especi ially the case for simple models such as the compound symmetry model.

Another important direction is $\mathbf{l}_{\max}$ which is the direction of maximal local influence. It indicates in what direction the MAR model should be extended in order to have maximal local changes in the likelihood. A small value for the corresponding influence measure $C_{\max}$ supports the MAR assumption while a large value for $C_{\max}$ indicates that the reason why some patients have dropped out is probably related to their unobserved outcome. In the latter case, model (1) should only be used if all components in $\mathbf{l}_{\max}$ are approximately the same, indicating that all dropouts are equally informative. If this is not the case, then a more elaborate model should be used, allowing for a mixture of dropout processes.

4 ANALYSIS OF MILK DATA

As an illustration, we have applied the above local influence approach to data on the occurence of infectious disease mastitis in dairy cows, which have been analysed by Diggle and Kenward [2] using an informative dropout model of the form (1). Later, Kenward [4] re-analyzed the data, and he noticed that removing two cows (with unusually small first measurement) shows complete lack of evidence for non-random dropout. This latter procedure is a global influence analysis since the effect is studied of completely removing two observations from the analyses. It is reassuring that our local influence procedure found the same cows to be influential, if the dropout mechanism is parameterized in terms of the increment from the first to the second measurement.

5 CONCLUSION

In this paper, we have shown how the impact can be studied of small perturbations around the null model of random dropout on the estimation of the parameters in the measurement model as well as in the dropout model. Further, the calculation of our influence diagnostics is very straightforward as it does not require fitting an informative dropout model. In general, local influence is to be preferred over global influence since it allows to assess direct and indirect influence on the dropout and measurement model parameters, while global influence procedures do not allow to disentangle the various sources of influence.

Clearly, other perturbation schemes than those applied here are worthwhile considering. However, not all schemes will lead to expressions that are both fairly easy to interpret and to calculate. Finally, the ideas outlined in this paper are not confined to the selection model of Diggle and Kenward [2], but can be extended to the pattern-mixture type and to models for categorical responses as well.

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SENSITIVITY TO LARGE-SCALE ENVIRONMENTAL FIELDS OF THE RELAXED ARAKAWA-SCHUBERT PARAMETERIZATION IN THE NASA GEOS-1 GCM

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1 INTRODUCTION

The GEOS-1 general circulation model (GCM) was developed by the NASA/GSFC/Data Assimilation Office and used in conjunction with their data assimilation system (DAS) to produce a multi-year global atmospheric dataset for climate research. In the physics packages of the GCM, the moist process plays an essential role towards improving the quality of the DAS products. The Relaxed Arakawa-Schubert (RAS) parameterization scheme [1] is the central part of this scheme.

RAS is a parameterization of sub-grid cumulus convection in terms of the large-scale fields. It is essential to evaluate its behavior regarding sensitivity to the large-scale environmental fields. Adjoint models provide an efficient tool to determine the sensitivity of certain measures of the model output (response function) with respect to perturbations in the model input variables and parameters (e.g., [2,3,4,5]). For RAS, important output quantities, directly relevant to model forecasts, are the time tendencies of potential temperature and specific humidity (moisture) of the surrounding air induced by the convective clouds, namely $(\frac{\partial \Theta}{\partial t})_c$ and $(\frac{\partial Q}{\partial t})_c$, respectively.

In this work the adjoint model of the GCM together with the adjoint of the RAS parameterization scheme [6] are used to analyze the sensitivity of RAS to large-scale fields. Some relevant issues to be addressed are: (i) the relative sensitivity of RAS to perturbations in Θ, Q and P_s fields of the surrounding air; (ii) the vertical and horizontal changes in sensitivity, as well as its regional changes; and (iii) the type of initial perturbations in the large-scale fields that significantly influence RAS.

This article is organized as follows. In Section 2, we briefly describe the theory and algorithm of adjoint sensitivity studies. Section 3 presents the result of the sensitivity analyses, and conclusions are drawn in Section 4.

2 ADJOINT SENSITIVITY METHOD

Let $\mathbf{x}$ be the GCM state vector, which incorporates the large-scale environment fields: winds, potential temperature, specific humidity and surface pressure, that is, U, V, Θ, Q and P_s, respectively. If $\mathbf{A}$ represents the RAS operator, a response function R of interest is

$$R = \int < \mathbf{A}(\mathbf{x},t), \mathbf{A}(\mathbf{x},t) >_{\mathbf{S}} \, dt \tag{1}$$

where $< \cdot\,, \cdot >_{\mathbf{S}}$ represents the inner product between two vectors and weighted by a real, symmetric matrix $\mathbf{S}$ specified according to the fields of interest. A small perturbation $\delta\mathbf{x}$ on the state vector causes a change δR in the response function that can be calculated by

$$\delta R = 2 \int < \widetilde{\mathbf{A}(\mathbf{x},t)}, \partial\mathbf{A}(\mathbf{x},t)\delta\mathbf{x} >_{\mathbf{S}} \, dt = 2 \int < \partial^*\mathbf{A}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t), \delta\mathbf{x} >_{\mathbf{S}} \, dt \tag{2}$$

with $\partial\mathbf{A}$ being the tangent linear operator of the RAS operator, and $\partial^*\mathbf{A}$ being its adjoint.

To determine the impact of small perturbations in the environment fields on R we need to evaluate its gradient with respect to $\mathbf{x}_0$. For that, we recall that small perturbations $\delta\mathbf{x}$ of the background fields evolve according to the GCM's tangent linear operator $\mathcal{L}$ as

$$\delta\mathbf{x} = \mathcal{L}(\mathbf{x}, t)\delta\mathbf{x}_0 \tag{3}$$

Defining $\mathcal{L}^*$ as the adjoint of $\mathcal{L}$, δR may be written as

$$\delta R \;=\; 2\int < [\mathcal{L}^*(x,t)\partial^*\mathbf{A}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)]dt, \delta\mathbf{x}_0 >_S \tag{4}$$

Therefore the gradient of R with respect to initial perturbation is given by

$$\nabla_{\mathbf{x}_0} R = 2\int [\mathcal{L}^*(x,t)\partial^*\mathbf{A}(\mathbf{x},t)\mathbf{A}(\mathbf{x},t)]dt \tag{5}$$

This gradient gives the optimal sensitivity patterns in the sense that for all the initial perturbations with unit norm, the one with the same spatial distribution as $\nabla_{\mathbf{x}_0} R$, i.e., parallel to $\nabla_{\mathbf{x}_0} R$, imposes the largest changes in R. In practice, the algorithm to calculate the gradient vector (5) is as follows:

1. Integrate the GCM from $t = t_0$ to $t = t_N$, saving the environment fields as well as the RAS output $[\mathbf{A}(\mathbf{x}, t)$ in (5)] at desired times t_n, for $n = 0, 1, 2, \ldots, N$;

2. At each time t_n, use the stored history of RAS [$\mathbf{A}(\mathbf{x},t)$] as input to its adjoint, to obtain the term $\partial^*\mathbf{A}(\mathbf{x}, t)\mathbf{A}(\mathbf{x}, t)$ in (5). At each step, we have the gradient of R with respect to instantaneous perturbations of the large-scale fields;

3. Finally, backward-integrate the adjoint of the complete GCM from t_N to t_0. Because $\mathcal{L}^*$ is linear, the result of step 2 can be added to the corresponding environment fields of adjoint GCM, at each t_n. The result at t_0 is $\nabla_{\mathbf{x}_0} R$ in (5).

The integration of the adjoint of the GCM, in step 3 above, yields the time evolution of sensitivity.

In what follows the weighting matrix S in (1) is chosen such that the following two response functions can be examined:

$$R_1 \;=\; \int \textstyle\sum_G (\frac{\partial\Theta}{\partial t})_c^2 dt \qquad R_2 \;=\; \int \textstyle\sum_G (\frac{\partial Q}{\partial t})_c^2 dt \tag{6}$$

for $\sum_G$ representing summation over selected grid points. These functions provide a measure of strength of the impact of convective clouds on the large-scale fields.

3 SENSITIVITY ANALYSIS RESULTS

Details on the atmospheric GCM can be found in [7]. The RAS scheme is the only physical process included in the integrations of the GCM, tangent linear and adjoint models, here (see [6], for details). All experiments were performed with $5° \times 4°$ resolution and 20 vertical layers. The integrations in time were carried out for 6 hours starting from 00GMT, 1 January 1985.

In Fig. 1 we show the longitude-height distribution of the R_2 sensitivity to temperature, where the gradient vector (5) is averaged in the latitude band between $10°S$ to $10°N$. Sensitivity is positive below 900hPa and negative at all upper levels. This indicates that a warming up of the sub-cloud layer and a cooling down of the upper layers favor convective activities and lead to strong convective drying of the whole column. The strongest positive and negative sensitivities are located at 950hPa and 600 hPa, respectively.

A longitude-height plot (not shown) of the R_1 sensitivity shows large resemblance to that for R_2, but without the secondary minimum around 800 hPa. Its strongest negative center is located at 500hPa, which is higher than what is seen in Fig. 1 for the R_2 sensitivity. This indicates that lower (higher) temperature at higher (lower) level tends to enhance convective heating to the surrounding air. In Fig. 2 the R_1 sensitivity at 500 hPa is shown. The distribution at other levels shows generally similar patterns.

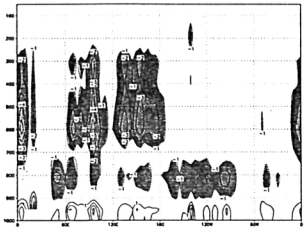


Figure 1: Longitude-height cross section of the R_2 sensitivity to temperature, averaged between $10°S$ and $10°N$.

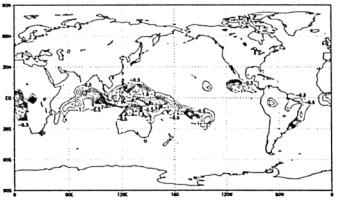
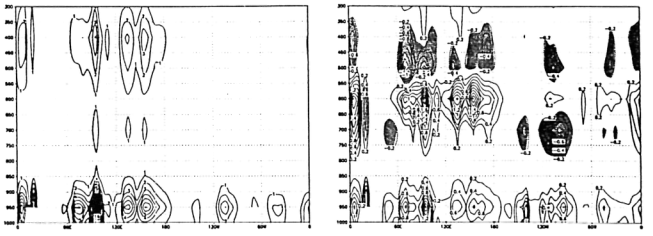


Figure 2: Latitude-longitude map of the R_1 sensitivity to temperature at 500 hPa.

We see from the figure that significant sensitivity is concentrated at low latitudes, with the strongest centers over the Indian and the west–central Pacific Oceans. The east Pacific convergence zone also appears to be relatively sensitive. These highly sensitive regions correspond to the ones with the most frequent and strongest climatological convective activities.

Figure 3 shows longitude-height maps of sensitivity to the moisture field. In Fig. 3a, for R_1, we see positive sensitivity at all levels, with a maximum at 950 hPa. This indicates that an overall increase in moisture tends to increase convective heating of the whole column, and that the moisture profile has a stronger impact on convection at the sub-cloud layer than at upper layers. The R_2 sensitivity to moisture in the surrounding air, seen in Fig. 3b, has the strongest positive (negative) sensitivity around 600hPa (500hPa). This distribution indicates that the moistening effect of convection is very sensitive to the moisture profile between 400hPa and 650hPa. When a positive moisture perturbation occurs at around 600 hPa, it enhances convective activity which in turn enhances convective drying. Therefore, there is a negative feedback between moisture and convection. On the other hand, when the moistening occurs above 500hPa, or so, there is tendency to suppress convective activity, leading to weak convective drying. In this case, there is a positive feedback between moisture and convective drying. The horizontal distribution of the R_1 and R_2 sensitivities to moisture is similar to that shown in Fig. 2 for sensitivity to temperature, except that at high levels, the R_1 sensitivity to moisture is positive instead of negative (not shown). The most sensitive area to moisture is again over the warm waters of Indian and western Pacific Oceans.



(a) (b)

Figure 3: As in Fig. 1, but for R_1 (panel a) and R_2 sensitivities (panel b) to moisture.

4 CONCLUSIONS

Perturbations in temperature and moisture fields have the most significant impact on RAS. The convective impact on the surrounding air is most sensitive to the temperature and moisture distribution at the sub-cloud layer as well as the layers between 500 and 600 hPa, at initial time. Warming of the sub-cloud layers and cooling of the upper layers tend to enhance convective heating of the surrounding air over the whole column. Moistening in the layers below 900hPa favors convective heating and moistening over the whole column. An increase of moisture in the mid-troposphere has little effect on convective heating, but it significantly enhances convective drying. Increasing moisture at levels above 500hPa leads to a increase of convective heating, and a decrease of convective drying. The effects of wind, surface pressure and model parameters will be discussed at the time of the conference.

The indications from this preliminary sensitivity results of the GEOS-1 RAS seem to be that accurate temperature and moisture data, especially over the convectively active regions over low latitudes are essential for the parameterization of the cumulus cloud effect to be accurately represented. It is expected that such data can significantly influence convective precipitation and other outputs of RAS. Better initial data, especially in those sensitive regions indicated in this work, may also improve the model spin-up during the the first several hours of a forecast.

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SENSITIVITY OF AN ELECTROSTATIC FIELD IN A CURVILINEAR CONDENSER AND OF ITS PROPERTY TO FOCUS CHARGE PARTICLES TO ELECTRODE DISTORTIONS

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A problem of tolerances, important for an adequate design and manufacturing of analytical instruments based on focusing and separation of charged particles in electrostatic fields, requires an investigation of a sensitivity of a particle beam behaviour to various types of distortions of electrodes that form this field. Generally the main part of this investigation, namely a study of the sensitivity of the electrostatic field distribution to electrode distortions, can be solved only by variance-based numerical algorithms, either differential, like a Bertein method [1], or integral, like a method of "integral equations in variations" by M.A.Monastyrsky [2]. From the mathematical point of view these methods adapt general numerical algorithms of solving the Laplace equation with some boundary conditions to the situation where the characteristic scales of the field region and of distortions of the boundaries of this region are very different. Being precise and versatile, such algorithms, however, do not provide for general relationships that describe in an analytical form an influence on the field structure of different typical boundary distortions.

In many analytical instruments charged particles move between two curvilinear electrode surfaces placed close by each other, so that the interelectrode gap of the condenser is smaller than the curvature radii. In these situations the sensitivity of the electrostatic field distribution and of its focusing propreties to electrode distortions can be investigated based on very simple and efficient asymptotic analytical approaches.

The first of these approaches can be called "a method of a direct substitution" of the Taylor expansion of the field potential into boundary conditions. We illustrate it on the example of the charged particle beam motion along the circular main path of the radius r_0 in a sector electrostatic condenser whose electrodes (generally toroidal) are separated by the gap $2b = 2\epsilon r_0$, where $\epsilon \ll 1$ is a small parameter. In such a toroidal condenser the electrostatic potential can be represented in a cylindrical coordinate frame $\eta = (r - r_0)/r_0$ and $\zeta = z/r_0$ as a Taylor expansion

$$U = \sum_{i,k=0}^{\infty} \frac{H_{ik}^{(n)}(\phi)}{i!k!} \eta^i \zeta^k \epsilon^n, \qquad (1)$$

where ϕ is an azimuthal angle. This expansion can be substituted into the Laplace equation $\Delta U = 0$ as well as into boundary conditions $U(\eta_j, \zeta, \phi) = V_j$ at the electrodes $j = 1, 2$ with the potentials V_j. Here $\eta_j = F_j(\zeta) + \epsilon f_j(\zeta, \phi)$ are equations defining boundary conditions, the functions F_j specifying their "perfect" parts and the functions f_j the electrode distortions. The substitution leads to a sequence of equations for the expansion coefficients of Eq. (1). Solving these equations, one can express in a form of asymptotic expansions with respect to the small parameter ϵ the Taylor coefficients $H_{ik} = H_{ik}^{(0)} + \epsilon H_{ik}^{(1)} + \ldots$ of the field distribution along the main beam path; the coefficients $H_{ik}^{(n)}$ are analytical functions of the functions f_j and their derivatives. Thus, for a given electrode distortion one can obtain a compact analytical formulae for the field variation.

Futhermore, the substitution of the resulting field representation of Eq. (1) into the Lorentz equations gives the charged particle trajectory representation in the form of aberration integrals, conventionally used in charged particle optics [3]. These integrals express the sensitivity of the particle beam shape to various electrode distortions.

The method of the direct substitution can be applied in case the electrode distortions are smooth. For sharp local distortions like scratches on the electrodes, another analytical approach can be applied. We illustrate it on the example of a long lateral scratch at the surface of the inner electrode of a cylindrical condenser with the electrode radii r_1 and r_2.

Let the defect be described by a local function $\rho(\phi)$ defined on a narrow interval of azimuthal angles $|\phi - \phi_0| < \epsilon$, that is the electrode surface on this interval be $r(\phi) = r_1[1 + \rho(\phi)]$. The derivative of the function $\rho(\phi)$ is not assumed to be small. There exists a conformal mapping of the band with the unity width to the region $r_1[1 + \rho(\phi)] < r < r_2$, $-\infty < \phi < \infty$. Though this mapping cannot be represented in an explicit form, one can obtain an analytical representation of its asymptotic expansion in the vicinity of the beam main path. This asymptotic expansion allows one to express approximately the variation of the electrostatic field potential δU caused by the scratch in the following form:

$$\delta U(r, \phi) = -\frac{(V_2 - V_1)Q}{2} \frac{\sin[B \ln(r/r_1)]}{\cosh[B(\phi - \phi_0)] - \cos[B \ln(r/r_1)]}, \tag{2}$$

where $B = \pi / \ln R$, $R = r_2/r_1$, V_1 and V_2 are electrode potentials. The sensitivity of the field structure to the scratch shape is determined in Eq. (2) by a parameter Q that can be estimated by various ways. In particular, a simple estimation in case of the scratch ($\rho(\phi) < 0$, $Q < 0$) is

$$|Q| \leq \frac{1}{R} \left| \int \rho(\phi_0 - x \ln R)\, dx \right|.$$

Particle trajectory distortions in the cylindrical condenser with a local defect can be, similarly to the case of a smooth electrode distortion, expressed in a form of aberration integrals. Moreover, assuming that the interelectrode gap of the condenser is small as compared with the electrode radii ($B \gg 1$), it is possible to obtain analytical asymptotic expressions for the beam distortions. In particular, the formulae that describes a lateral shift g of the beam main path at the exit of the condenser (corresponding to the azimuthal angle ϕ_e), takes a very simple form

$$g = -\frac{Q}{\sqrt{2} \ln R} \sin \sqrt{2}(\phi_e - \phi_0).$$

Thus asymptotic approaches allow one to simplify considerably the investigation of the sensitivity of the electrostatic field structure in a curvilinear condenser as well as of the charged particle beam transport through this condenser to manufacturing imperfections of the electrodes.

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SIMPLICITY OUT OF COMPLEXITY: DATA-BASED MECHANISTIC MODELLING, GENERALISED SENSITIVITY AND DOMINANT MODE ANALYSIS

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1 INTRODUCTION

Bearing in mind the inherent uncertainties associated with the modelling of environmental and climate systems, it seems sensible to consider alternative modelling methodologies which overtly acknowledge the often poorly defined nature of such systems and the need to better understand the kind of large, deterministic models that characterise much environmental modelling and climate research. This paper considers the Data-based Mechanistic (DBM) approach to modelling and discusses two approaches to the analysis and simplification of large simulation models that can be considered within this general philosophical framework: Generalised Sensitivity Analysis (GSA) based on Monte-Carlo Simulation (MCS); and Dominant Mode Analysis (DMA), in which a simplified model is obtained by a new statistical approach to combined model linearisation and order reduction. Details of each approach are given, together with a review of their application to the analysis of nonlinear global carbon cycle models.

2 DATA-BASED MECHANISTIC (DBM) MODELLING

In DBM modelling (see [1],[2],[3]), the aim is to statistically identify and estimate a 'data-based' model of a stochastic, dynamic system that can be interpreted in physically meaningful terms. This normally results in a low order, parametrically efficient and well estimated model which is not overly constrained by the prior perceptions of the modeller. This DBM approach has been applied successfully to various environmental, biological, ecological, engineering and economic systems ([4]). In this paper, however, we will consider its *less* successful application to global climate data. In the case of the relationship between global fossil fuel input and atmospheric carbon dioxide, for example, the DBM analysis yields a second order linear model composed of two, serially connected, first order processes which explains 99.8% of the data. On the other hand, it is difficult to place any clear mechanistic interpretation on this model and it can be argued (although we do not necessarily take this view) that the simplicity of the identified model is due more to the lack of information in the data than to the simplicity of the dynamics associated with the global climate system. Consequently, it makes sense to consider alternative and more complex simulation models that have greater inherent descriptive and explanatory potential. But, if it is to be successful, this alternative must be based on an approach which acknowledges the deficiencies of large simulation models. Such an approach is considered in the subsequent sections of the paper.

3 STOCHASTIC (MONTE CARLO) SIMULATION MODELLING

Young [5] has argued that stochastic modelling is a powerful tool for investigating poorly defined systems with limited observational data, such as the global climate. However, it is an approach which is rarely used in climate research, possibly due to the reductionist view that it is 'second best' [6]. In contrast, our studies have shown that stochastic modelling can enhance deterministic simulation modelling and provide a useful technique for both evaluating the effects of uncertainty in the system and defining the most significant parameters in the model. This is achieved by converting the physically-based, deterministic simulation model into stochastic form by assuming that its parameters and inputs are inherently uncertain: the parameters being characterised by probability density functions (pdf's); and each input being expressed in terms of a stochastic time series model.

Adopting a Bayesian approach, the pdf's are defined by reference to the current scientific literature on the parameter values and their associated uncertainty. The subsequent analysis then exploits Monte Carlo Simulation (MCS): i.e. the repeated simulation of the model, with the parameter and input values for each simulation run (or 'stochastic realisation') randomly drawn from the defined pdf's. Typically, MCS involves several hundred, and sometimes several thousand, simulation runs: the exact number being dependent on the

required accuracy of the output statistical measures, such as cumulative distribution functions for each output variable (e.g. [7]).

Using this MCS methodology, the effects of uncertainty have been examined for a 23rd order, nonlinear global carbon cycle model (EL: [8]) that has figured in the deliberations of the International Panel on Climate Change (IPCC). Typical results show that the uncertainty in the model response is far greater than that in the observations. In addition, a special form of GSA (e.g. [7],[9]) based on MCS reveals that the E-L model is quite sensitive to the values of certain statistically significant parameters, especially the pre-industrial level of atmospheric CO_2. The stochastic uncertainty propagation in the E-L model is also much larger than the range of outputs generated in deterministic model scenario studies, such as those obtained using the well known STUGE model of Wigley and Raper, [10].

In total, these comprehensive and objective MCS results suggest quite strongly that the presence and effects of uncertainty are not at present being considered adequately by many climate modellers. This is not too surprising in the case of Global Circulation Models (GCM's), since their huge computational demands appear to preclude Monte Carlo uncertainty analysis. But the omission is still a weakness which limits any objective assessment of GCM results in relation to the uncertainty which should be an essential aspect of any exercise in global modelling [11].

4 DOMINANT MODE ANALYSIS (DMA)

DMA seeks to analyse a given, physically-based, deterministic model by identifying the small number of dynamic modes which appear to dominate the model's response to perturbations in the input variables. In contrast to traditional reductionist modelling this normally results in a considerable simplification of the model structure rather than an increase in complexity. The methodology involves perturbing the complex and usually nonlinear, physically-based simulation model about some defined equilibrium or operating point, using a *sufficiently exciting* signal, i.e. one that will unambiguously reveal all the dominant modes of behaviour (see [7]). A low order, linear model, in the form of a transfer function (in any one of the standard operators: backward shift, delta or differential), is then fitted to the resulting set of simulated input-output data, using special methods of statistical identification and estimation that are particularly effective in this role (see [12],[13] for more details). As might be expected from dynamic systems theory, a low order linear model obtained in this manner reproduces the quasi-linear behaviour of the original nonlinear model about the operating point almost exactly for small perturbations. Perhaps more surprisingly, however, the dominant mode model can sometimes also mimic the large perturbation response, as it does in the case of the E-L model.

To carry out the DM analysis, the full nonlinear E-L model is initially set to an equilibrium condition with an atmospheric CO_2 concentration of 275 ppmv. Then perturbations in the fossil fuel input are applied to the model and the resulting responses are monitored over a period of 3000 years. The statistical identification and estimation analysis (see [7]) yields a 4th order, linear transfer function model which explains 99.98% of the physically-based model perturbations. More significantly still, it also reproduces the behaviour of the 23rd order nonlinear model over the entire industrial period: here, the error is always very small, never greater than 0.5 ppmv, even though the model has moved 45 ppmv above the operating point at which it was estimated.

These results demonstrate the robustness of the low order, dominant mode model and suggest that the non-linearities in the original model are hardly being excited by these fairly substantial perturbations over the industrial period. Moreover, further DMA results at a range of different operating points reveal that the objectively identified, 4th order model structure does not change at all, and the behaviour of the nonlinear model can be reproduced very closely with only small variations in the parameter values.

More recently, the same approach has been applied to another global carbon cycle model: the *ANU-BACE* model developed in the Centre for Resource and Environmental Studies at the Australian National University. Here again, it has been possible to obtain a low order (this time 5th order) linear differential equation model which mimics well the behaviour of the high order nonlinear model over the historical period.

5 CONCLUSIONS

All three of the modelling methodologies outlined in this paper and discussed in detail by Young et al [7] are still being developed and have their limitations. Nevertheless, they offer useful additions to conventional deterministic and reductionist approaches, with considerable potential for revealing new information and insight within the area of environmental and climate modelling (and, indeed, in other fields: see [4]). The results

presented here help to emphasise that the large, deterministic, simulation models that are so popular in environmental and climate research can have many limitations and are not the *only* type of model that should be considered, particularly when there are uncertainties, or even ambiguities, in both our scientific knowledge of system under study and the observational data base. And when such large, deterministic models are used in uncertain situations, the model developers should *overtly* recognise the presence of uncertainties and over-parameterisation, attempt to quantify these aspects of the model, and then take account of them in both the development and use of the models [11].

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APPLICATION OF SENSITIVITY ANALYSIS TO ENVIRONMENTAL MANAGEMENT

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1 INTRODUCTION

Environmental management is essentially conflict analysis characterized by technical, socio-economic, environmental and political value judgments. This is due to the fact that several stakeholder groups, technical as well as non-technical, are typically involved in the task of managing environmental programs. These groups tend to support their own, diverse, objectives and values. In particular, due to increased environmental concern and awareness of environmental risks, the public demands to be involved in decisions that may affect their health and environment, and which require the use of public money. Consequently, in an environmental planning process it is very difficult to arrive at straigtforward and unambiguous solutions but, rather, acceptable compromise solutions need to be searched for, an activity which requires an adequate and comprehensive evaluation methodology.

In this context, a methodology for evaluating environmental restoration technologies using integrated risk communication, assessment, and management tools has been developed. This methodology consists of two main parts: the first part ("analysis") integrates a wide range of decision criteria and impact evaluation techniques in a framework that emphasizes and incorporates input from stakeholders in all aspects of the process. Its products are the rankings of the alternative options for each stakeholder using, essentially, expected utility theory. The second part ("deliberation") utilizes the analytical results of the "analysis" and attempts to develop consensus among the stakeholders in a session in which the stakeholders discuss and evaluate the analytical results. This paper deals with the analytical part of the approach and the sensitivity analyses that were carried out in preparation for the deliberative process.

2 A METHODOLOGY FOR ENVIRONMENTAL MANAGEMENT WITH MULTIPLE STAKEHOLDERS

The first step of the methodology is that of identifying all consequences relevant to the implementation of the decision, i.e. the performance measures. These are identified through a decomposition process which allows the subdivision of the issues of interest in their constituent components. The process is based on the use of conditional influence diagrams to incorporate and structure the quantitative and qualitative issues of the decision problem [1].

Aggregation of the evaluations of the performance measures is done by means of an additive utility function (*performance index*), viz.

$$u(\underline{x}) = \sum_{k=1}^{N_{pm}} w_k u_k(x_k) \qquad (1)$$

where w_k, the priority weight of the k-th performance measure, $k=1,2, \ldots, N_{pm}$, gives an indication of the relative importance of the performance measure, u_k is the single-attribute utility function for performance measure k, and x_k is the associated consequence variable.

The weights are assessed by the pairwise comparison method of the Analytic Hierarchy Process [2] applied to the hierarchical structure of the influence diagram. With respect to the classical methods of defining trade-offs in utility theory, this method has the advantage that pairwise comparison judgments are easy to elicit and the weights w_k of the performance measures synthesize the information contained in all possible pairwise comparisons among them. The redundancy of this information contributes to the robustness of the estimates and allows for a considerable degree of control over inconsistent judgments.

For the determination of the single-attribute utilities we employ a direct approach based on the AHP combined with elements of fuzzy logic [3]. The main idea is to split the range of the performance measure in three subranges of performance: *worst*, *moderate* and *best*. These are defined as the ranges of consequence values which are considered respectively as least, average and most preferred, by the stakeholder. For example, a stakeholder may consider the cost of implementation of remediation technologies "worst" when it costs more

than five million dollars, "moderate" if it is within one and five million, and "best" if it is less than three million dollars. Note how these sets need not necessarily be exclusive.

For a given performance measure the utility function should then be such that, if an alternative gives an outcome which falls in the "worst" range, it should receive a low utility value in accordance to the preference attitude of the stakeholder. On the contrary, if the outcome for that alternative falls within the "best" range, it is preferred by the stakeholder and this should be reflected in a high utility value. An outcome in the "moderate range" is moderately satisfactory for the stakeholder and thus should receive a moderate value of utility.

However, concepts such as "worst", "moderate" and "best" consequences are far from being universal and clearly defined; indeed, it is expected that every stakeholder will have a different perception of these concepts. To account for such linguistic imprecision, appropriate membership functions are introduced. We are then dealing with performance measures extending over fuzzy ranges.

A thorough analysis of the results obtained for each stakeholder allows us to gain insights into the reasons behind the differences in the preferences for the various options. These insights provide focused, transparent arguments for an open deliberative process aiming at achieving a fair and wise decision.

The prototype methodology was tested on a case study regarding the selection of one out of six remediation action alternatives (RAA A through F). The analysis involved six different stakeholders (SH1 through SH6) representing different concerns, perspectives and backgrounds.

3 SENSITIVITY ANALYSIS

An important part of the process is sensitivity analysis which investigates how the rankings of the alternative actions change when the inputs to the decision analysis differ from the best estimate values. The importance of such an investigation is two-fold. First, before the rankings resulting from the decision process are accepted, one must always confirm the robustness and stability of the findings.

Secondly, the results of the sensitivity analysis may help to reveal the sources of disagreements among stakeholders. For example, in the "Participatory Group Decision Model" proposed by Keeney and Raiffa [4], where consensus on the weighting factors of a multiattribute utility analysis is needed, sensitivity analysis is explicitly indicated as a means to seek for agreement.

In our model for decision making, (eq. 1), the input quantities which directly affect the performance index outputs are the single-attribute utilities $u_k(x_k)$ and the weights w_k.

The main source of variability of the single-attribute utilities comes from the uncertainty in the consequences x_k. This uncertainty is obviously not subjective but, rather, factual and, therefore, its analysis does not provide any insight on the sources of disagreements among stakeholders; still, robustness of the results must be tested. Indeed, an uncertainty analysis showed that the uncertainty in the output is, in general, contained so that the final rankings based on the performance indices (utilities) of each alternative are rather stable for all stakeholders (Figure 1).

On the other hand, the subjective and uncertain character of the weight assignments by the stakeholders to the various issues and objectives considered in the decision process calls for a detailed sensitivity analysis on the weight variability, both for testing of the robustness of the results and for searching points of agreement and disagreement at different levels.

Several formal approaches have been developed for performing sensitivity studies [5]. Of these approaches, a combination of differential analysis, based on Taylor's expansion, followed by a Monte Carlo sampling, focused on the most important input variables as identified by the differential analysis, was applied to evaluate the effects of changes in the objective categories, objectives and performance measures priority weights on the ranks of the action alternatives.

The differential analysis on the weights confirmed the indications on the main driving performance measures obtained in a previous analysis on the utilites of each stakeholder.

For the Monte Carlo analysis, the ranges of the weights at a given level of the hierarchical structure were chosen in such a way as to maintain the order of the rankings within that level. For instance, if we have the following weights: w_1=0.6, w_2=0.3, w_3=0.1, we can perform sensitivity runs to investigate the influence of w_2 values between, say, 0.101 and 0.599, which represent the range that maintains the ranking, and re-normalizing all the weight values to unity. The sensitivity analysis on this nominal range is then performed by varying each input weight in turn. In this manner, the weights for which the choice of values actually change which decision alternative is preferred can be identified and the uncertainty on their values can be accounted for.

Given the two or three most important variables as determined by the sensitivity analysis, a policy region analysis can be performed [6]. This involves varying simultaneously the most important weights over their entire ranges and shows which decision alternative is preferred over these ranges.

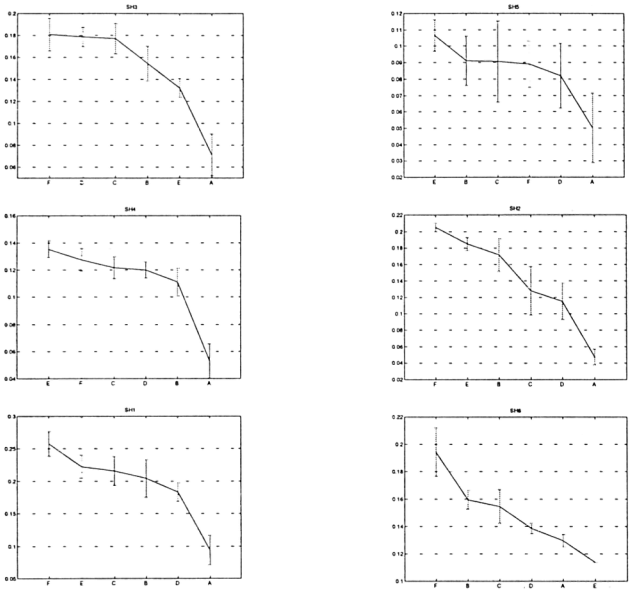


Figure1: Uncertainty bands for the performance indices (utilities) of the remediatiation action alternatives

The results of the sensitivity and policy region analyses for all stakeholders showed that, in most cases the rankings of the alternatives are highly stable and robust, and provided some interesting insights regarding the stakeholders preference structure.

For stakeholder SH5, for example, it can be seen that, as the weight on the performance measure *worker health risk* (*xwhr*) is increased relative to the others, within its range of variability, F soon becomes the second preferred option after E and tends to outperform it (Figure 2). A similar effect is found when varying the weight of the performance measure *implementation costs* (*xic*) up to a value equal to that of the other cost-related performance measure, *completion costs* (Figure 3), although in this case B results as the most preferred alternative, with F a close second.

For SH4, analogous considerations can be made for the variation of the weight on the objective category *worker health risk* (*xwhr*) within its range of variability and of the weight of the objective category *life cycle cost* (*xlcc*). A two-way policy region analysis on alternatives F and E with respect to *xwhr* and *xlcc*, confirms the existence of a region of high importance of worker health risk (of the order of that obtained from the stakeholder input) and high importance of life cycle cost (approximately double of that obtained from the stakeholder inputs) where alternative F is preferred to E (Figure 4).

These results provide valuable insights on the levels of agreement among stakeholders, and of compromise which can be sought for, and constitute key elements in the process of consensus building which is the objective of the successive deliberation phase of the methodology.

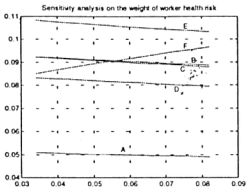


Figure 2: Sensitivity of the performance indices to changes in the weight of worker health risk (xwhr)

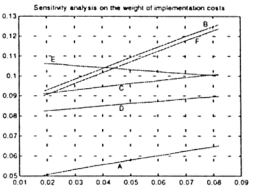
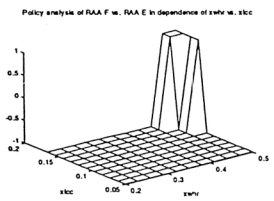


Figure 3: Sensitivity of the performance indices to changes in the weight of implementation costs (xic)



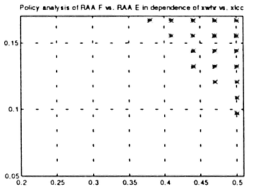


*Figure 4: A two-way policy region analysis for the variables xwhr and xlcc and decision alternatives E and F: in the 3D figure, +1=RAA F preferred to RAA E; -1=RAA E preferred to RAA F; in the 2D figure *=RAA F preferred to RAA E.*

4 CONCLUSIONS

A methodology for evaluating environmental restoration technologies has been developed and demonstrated on a real case study.

This paper illustrates an important phase of the methodology, sensitivity analysis, which investigates how the rankings of the alternative remediation actions change when the inputs to the decision analysis differ from the best estimate values. In particular, we have focussed our attention on the variability of the subjective importance weight assignment to the various issues of concern in the decision context.

This analysis allows testing of the robustness and stability of the results obtained and provides significant insights which have proven useful for the successive deliberative phase of the process in which the stakeholders are asked to reach a reasonable degree of consensus on potential recommendations to the regulatory agency on the implementation of a remediation technology.

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