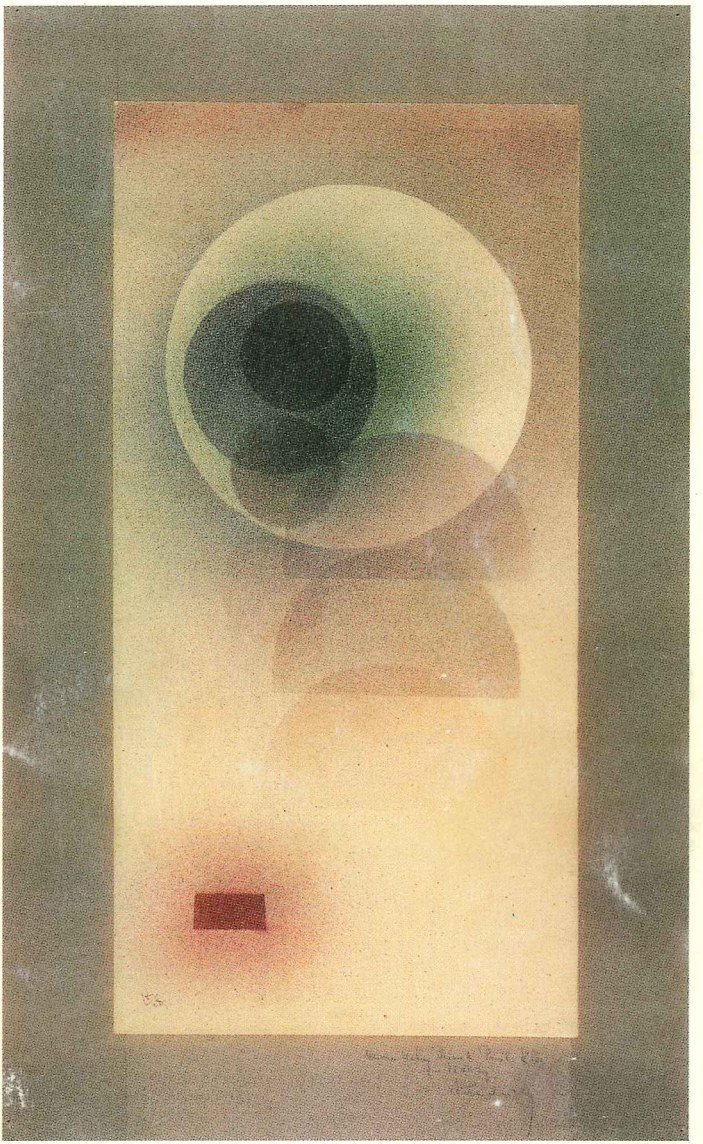

SAMO 95

Theory and applications of Sensitivity Analysis of Model Output in computer simulation

25th-27th September 1995 Belgirate-Italy

Organised by: European Commission DGXII/F - RTD Action Energy - Joint Research Centre, Environment Institute

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25th-27th September 1995 Belgirate-Italy

PROGRAMME AND EXTENDED ABSTRACTS

Organised by: European Commission DGXII/F - RTD Action Energy - Joint Research Centre, Environment Institute

Programme

MONDAY 25 September 1995

08.30 Welcoming Address from R.H. Von Maravic
European Commission DG XII

MONDAY 25 Morning Sessions

Session **Subjective versus stochastic uncertainty**

Chairman: S.C. Hora

08.40 J.C. Helton, Invited paper
(Dept. of Mathematics, Arizona State Univ., Tempe, USA)
Uncertainty and Sensitivity analysis in the presence of stochastic and subjective uncertainty

09.10 T. Zimmerman, Ghislain de Marsily, S. Gorelick, M.G. Marietta and C. Axness
(GRAM Inc. of Albuquerque, Univ. of Paris, F, and SANDIA Laboratory, USA)
The sensitivity of models of groundwater flow to conceptual model uncertainty and its importance in radionuclide transport problems

Session **Sampling strategies and parameter screening**

Chairman: I.M. Sobol'

09.30 T.H. Andres, Invited paper
(AECL CANADA, Whiteshell Establishment, Pinawa, Manitoba, CAN)
Sampling methods and sensitivity analysis for large parameter sets

10.00 S.C. Bankes, T.W. Lucas
(RAND, Santa Monica, CA, USA)
Statistical approaches for the exploratory modelling of large complex models

10.20 Coffee break

10.50 N. Rahni, N. Ramdani, Y. Candau and P. Dalicieux
(Univ. of Paris XII and EDF of Moret-sur-Loing, F)
Sensitivity analysis of dynamic buildings energy simulation models using group screening and sampling methods

11.10 T. Bedford, A.M.H. Meeuwissen
(Faculty of Mathematics of Delft, and PTT Research Laboratory, Leidschendam, NL)
The determination of maximum entropy distributions given fixed rank correlation, and numerical approximations for use in sensitivity analyses

Session Sensitivity analysis in perspective

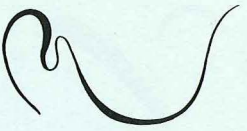
Chairman: J.C. Helton

11.30 J.P.C. Kleijnen, Invited paper
(Department of Economics of the Tilburg University, NL)
Sensitivity analysis, uncertainty analysis, and validation. A survey of statistical techniques and case studies

12.00 E. Hofer, B. Krzykacz, Invited paper
(Gesellschaft für Anlagen-und Reaktorsicherheit (GRS) mbH, D)
On benefits and drawbacks of customary sensitivity measures

12.30 End of Morning Sessions

MONDAY 25, Afternoon Sessions



Session Sensitivity analysis in perspective continued

14.00 T. Turanyi, Invited paper
(Central Research Institute for Chemistry, Budapest, H)
Applications of sensitivity analysis to combustion chemistry

Session Global sensitivity measures

Chairman: J. Cawlfield

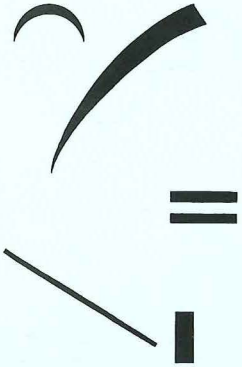
14.30 I.M. Sobol', Invited paper
(Institute for Mathematical Modelling of the Russian Academy of Science, Moscow, CIS)
Sensitivity analysis of nonlinear models using sensitivity indices

15.00 I.M. Sobol', A.L. Gershman
(Institute for Mathematical Modelling of the Russian Academy of Science, Moscow, CIS)
On an alternative global sensitivity estimator

15.20 T. Homma, Invited paper
(Institute of Nuclear Safety Nuclear Power Engineering Corporation, Tokyo, J)
Global sensitivity analysis in nuclear safety problems

15.50 Coffee break

16.20 A. Saltelli
(Environment Institute, European Communities, Joint Research Centre of Ispra, I)
On the use of rank transformation in sensitivity analysis



Session Local sensitivity methods in chemistry. Theory and applications

Chairman: D. Liepmann

16.40 A. Sandu, G.R. Carmichael, F.A. Potra
(University of Iowa, Iowa City, USA)
Sensitivity analysis for atmospheric chemistry models via automatic differentiation

17.00 H. Rabitz, Invited paper
(Dept. of Chemistry, Princeton University, New Jersey, USA)
Identification of critical variables and functions in chemical systems

17.30 F. Strozzi, V. Calenbuhr, M.A. Alos and J.M. Zaldivar
(Institute for Safety Technology, European Communities, Joint Research Centre of Ispra, I)
Sensitivity analysis using Lyapunov exponents; application to chemical reactors

17.50 G. Wotawa, A. Stohl and H. Kromp-Kolb
(Inst. for Meteorology and Physics, Univ. of Agric., Vienna, A)
Estimating the uncertainty of a Lagrangian photochemical air quality model (PAQSM) caused by inexact meteorological data

18.10 End of first day

TUESDAY 26, Morning Sessions

Session — The nuclear fuel cycle: sensitivity analisis in performance assessment and risk analysis

Chairman: G. Volta

08.30 J. Marivoet, P. Escalier des Orres, J.M. Gomit, J. Wibin, J. Prij and K.H. Marten, Invited paper (CEN/SCK Mol, B, CEA-IPSN, Fontenay-aux-Roses, F, ECN Petten, NL, and GRS Köln, D)
The EVEREST project. Sensitivity analysis of geological disposal systems

09.00 J. Andersson, B. Dverstorp, C. Lilja, K. Pers, B. Sundström, S. Wingefors (Office of Nuclear Waste Safety, Swedish Nuclear Power Inspectorate, and Kemakta Consultants, Stockholm, S)
Sensitivity of radionuclide release and transport to uncertainty and variability in properties of deep cristalline rock

09.20 B.C.P. Kraan, R.M. Cooke (Delft University of Technology, NL)
Joint CEC/USNRC post processing for uncertainty analysis

09.40 G. Prabhakar Rao, P.K. Sarkar (H.P. Unit, V.E.C. Centre, Calcutta, India)
Sensitivity studies of air scattered neutron dose from particle accelerators

10.00 P.K. Sarkar, H. Rief (Institute for Safety Technology, European Communities, Joint Research Centre of Ispra, I)
Differential operator sampling for self optimising Monte Carlo simulations

10.20 C. Ekberg, I. Lundén-Burö (Dept. of Nucl. Chemistry, Chalmers University of Technology, Göteborg, S)
Uncertainty analysis for some actinides at groundwater conditions

10.40 Coffee break

11.00 A. de Crécy
(French Atomic Energy Commission, Grenoble, F)
Determination of the uncertainties of the input parameters and sensitivity analysis on the CATHARE 2 code

11.20 R. Bolado, J.A. Moya and A. Alonso
(Nuclear Technology Chair, Polytechnic Univ. of Madrid and NEXUS5, Madrid, E)
MayDay. A code to perform uncertainty and sensitivity analysis. An application to 129Iodine in PSACOIN Level E exercise

Session Modelling sensitivities in decision analysis

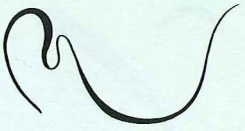
Chairman: J.P.C. Kleijnen

11.40 S.C. Hora, Invited paper
(University of Hawaii at Hilo, USA)
Sensitivity, uncertainty, and decision analyses in the prioritization of research

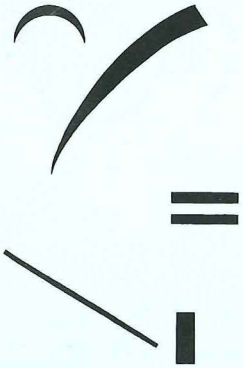
12.00 S. French, J. Martin, L. Proll, D. Rios Insua, A. Salhi
(University of Leeds, UK, University of Edinburgh, UK and Madrid Polytechnic University, E)
Sensitivity analysis in decision analysis

12.20 End of Morning Sessions

TUESDAY 26, Afternoon Sessions



Session	Innovative applications; SA in economics, energy management, epidemiology and other
	Chairman: S.C. Hora
14.00	W.J.H. Van Groenendaal, J.P.C. Kleijnen, Invited paper (School of Management and Economics, Tilburg University, NL) **Economic risk versus technological risk in large investment projects**
14.30	M.S. de Wit (Department of Civil Engineering, Technical University of Delft, NL) **Uncertainty analysis in building thermal modelling**
14.50	C. Bianchi , G. Bruno, A. Cividini (University of Pisa and Banca d'Italia, I) **Detecting the reliability of influential variables in the simulation of large nonlinear econometric models**
15.10	A.W. Jalvingh, M.W. Stern, A.A. Dijkhuizen and R.S. Morris (Wageningen Agricultural University, NL and Massey University, New Zealand) **Modelling the technical and economic consequences of control strategies for Foot-and-Mouth disease outbreaks in the European Union**
15.30	Coffee break
16.00	A.W. Lees (Berkeley Technology Centre, Nuclear Electric plc., Berkeley, Gloucerstershire, UK) **The sensitivity of force estimation in flexibility supported machines**



Session Exploring new concepts

Chairman: T. Turanyi

16.20 A. Gandini, J.-M. Gomit
(ENEA, Rome, I, and IPSN, Fontenay-aux-Roses, F)
The GTP methodology. New fields of application

16.40 T. Reilly
(Dept. of Decision Science, University of Oregon, Eugene, USA)
The effect of correlated variables on a one-way sensitivity analysis

17.00 K.-P. Huber, H. Szczerbicka and R. Barton
(University of Karlsruhe, and University of Bremen, D)
Locating sensitive regions by learning from simulation data

17.20 End of second day

18.00 Coctail and musical entertainment with the "*Insieme strumentale Romano*" and musics of W.A. Mozart

19.30 Conference dinner

WEDNESDAY 27, Morning Session

Session — Sensitivity analysis in presence of stochastic variation

Chairman: M. Scott

08.30 M. Koda, Invited paper
(IBM Research, Tokyo Lab., J)
Stochastic sensitivity analysis and Langevin simulation for neuronal network learning

09.00 A. Russo, P.D. Falorsi, S. Falorsi
(University of Molise and Italian Statistical Institute, I)
Sensitivity analysis of results of variation in the sampling error in the context of repeated sample survey

09.20 M. Di Traglia
(University of Molise, I)
Sensitivity analysis in the space-time statistical models

09.40 R.C.H. Cheng , W. Holland
(Inst. of Mathematics and Statistics, University of Kent at Canterbury, UK)
The sensitivity of computer simulation experiments to errors in input data

Session — Environmental modelling

Chairman: H. Rabitz

10.00 M. Scott, Invited paper
(Dept. of Statistics, University of Glasgow, UK)
Testing and assessment of environmental models

10.30 Coffee break

11.00 D. Liepmann, W. Chang, Invited paper
(Dept. of Mechanical Engineering, University of California, Berkeley CA, USA)
Application of FAST to a closed ecosystem model

11.30 F. Campolongo, A.J. Gabric
(Faculty of Environmental Sciences, Griffith University, Nathan, Australia)
The parametric sensitivity of the sea-to-air flux of dimethylsulphide in the southern ocean

11.50 R. Pastres, D. Franco, D. Pecenik, G. Solidoro and C. Dejak
(Dept. of Phys. Chem., University of Venice, I)
First order sensitivity analysis of distributed parameter ecological model

Session Sensitivity analysis methods in hydrology

Chairman: ~~J. Andersson~~

12.10 J. Cawlfield, Ming-Chee Wu, J.H. Piggot and S. Boatening, Invited paper
(Dept. of Geological and Petroleum Engineering, University of Missouri - Rolla, USA)
Probabilistic sensitivity measures as applied to saturated and unsaturated flow and transport

12.40 A.M. Riddle, R.J. Murray-Smith
(Brixham Environ. Laboratory, Zeneca Ltd., Freshwater Quarry, Devon, UK)
Uncertainties in modelling water flows through fractured rock

13.00 J. Devooght, O.F. Smidts
(Faculty of applied sciences, Free University of Brussels, B)
A variational method for determining uncertain parameters and geometry in hydrogeology

13.20 End of Symposium

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Scientific Committee

UNCERTAINTY AND SENSITIVITY ANALYSIS IN THE PRESENCE OF STOCHASTIC AND SUBJECTIVE UNCERTAINTY

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Tempe, AZ 85287-1804 USA

ABSTRACT

An assessment of the effects of uncertainty is widely recognized as an essential part of most analyses. Such assessments are typically subdivided into the related areas of uncertainty analysis and sensitivity analysis, where uncertainty analysis involves determining the uncertainty in model predictions that results from imprecisely known analysis inputs and sensitivity analysis involves determining the contribution of individual analysis inputs to the uncertainty in model predictions.

When viewed formally, many analyses consist of the following components:

$$\mathbf{x} = \text{a vector of inputs to the analysis,} \tag{1}$$

$$F = \text{a function of } \mathbf{x}, \tag{2}$$

$$(S, \mathcal{b}, \mu) = \text{a probability space that characterizes the uncertainty in } \mathbf{x}. \tag{3}$$

In this context, uncertainty analysis involves the determination of the complementary cumulative distribution function (CCDF) that derives from F and $(S, \mathcal{b}, \mu)$, and sensitivity analysis involves the determination of the contribution of the individual components of $\mathbf{x}$ to the uncertainty characterized by this CCDF.

In concept, uncertainty analysis is straight forward as it simply involves evaluation of the integral

$$prob\,(r > R) = \int_S \delta_R[F(\mathbf{x})]\, p(\mathbf{x})\, dV \tag{4}$$

where

$$\delta_R(r) = \begin{cases} 1 \text{ if } r > R \\ 0 \text{ if } r \le R \end{cases} \tag{5}$$

$$p(\mathbf{x}) = \text{density function for } (S, \mathcal{b}, \mu) \tag{6}$$

and *prob* ($r > R$) is the probability that the function (i.e., model) F will yield a prediction greater than R. Once evaluated, the preceding integral provides a complete characterization of the uncertainty in F. In practice, this evaluation is not simple at all as $\mathbf{x}$ is often of high dimension and F can be very complicated (e.g., a computer program consisting of 10^5 or more lines of FORTRAN).

A number of uncertainty analysis techniques have been developed to provide approximations to the information associated with the integral in Eq. (4), including differential analysis, the fast probability integral, the Fourier amplitude sensitivity test (FAST), Monte Carlo analysis, and response surface methodology (RSM). Each of the preceding procedures for approximating the integral in Eq. (4) also has associated measures of sensitivity. For example, sensitivity can be defined by fractional contribution to variance (differential analysis, FAST, Monte Carlo, RSM), regression models relating $F(\mathbf{x})$ to $\mathbf{x}$ (Monte Carlo, RSM), correlation analysis (Monte Carlo, RSM) and pattern identification (Monte Carlo). More complex procedures based on determination of the total impact of individual elements of $\mathbf{x}$ on $F(\mathbf{x})$ are also possible.

The focus of this presentation is analysis problems in which the probability space (S, $\mathcal{s}$, μ) in Eq. (3) is built up from two distinct probability spaces (S_1, $\mathcal{s}_1$, μ_1) and (S_2, $\mathcal{s}_2$, μ_2). Then $S = S_1 \times S_2$, $\mathcal{s} = \mathcal{s}_1 \times \mathcal{s}_2$, and μ characterizes the probabilistic relationships between S_1 and S_2. As an example, problems of this type often arise in performance assessments for complex systems, where one probability space is used to represent the possible occurrences that could take place in the system under study (i.e., stochastic or aleatory uncertainty), and the other probability space is used to represent uncertainty in the appropriate values of parameters to use in the computational implementation of the analysis (i.e., subjective or epistemic uncertainty).

When an element of one probability space is fixed (e.g., $\mathbf{x}_2 \in S_2$), then a CCDF results that characterizes the uncertainty in F due to the possible values that $\mathbf{x}_1 \in S_1$ can take on. Such CCDFs are defined by integrals of the form

$$prob\,(r > R \mid \mathbf{x}_2) = \int_{S_1} \delta_R\left[F(\mathbf{x}_1,\mathbf{x}_2)\right] p\,(\mathbf{x}_1|\mathbf{x}_2)\, dV_1, \tag{7}$$

where

$$p\,(\mathbf{x}_1|\mathbf{x}_2) = p\,(\mathbf{x}_1,\mathbf{x}_2) / \int_{S_1} p\,(\mathbf{x}_1,\mathbf{x}_2)\, dV_1 \tag{8}$$

$$p\,(\mathbf{x}_1,\mathbf{x}_2) = \text{density function for } (S, \mathcal{s}, \mu),\ S = S_1 \times S_2 \tag{9}$$

and *prob* ($r > R \mid \mathbf{x}_2$) is the probability that F yields a prediction greater than R conditional on the element $\mathbf{x}_2$ of S_2.

Three interrelated questions arise in uncertainty and sensitivity analyses that involve a product space $(S, \mathcal{S}, \mu)$ derived from two distinct probability spaces $(S_1, \mathcal{S}_1, \mu_1)$ and $(S_2, \mathcal{S}_2, \mu_2)$: How to estimate the individual CCDFs defined by the integrals in Eq. (7)?, How to estimate the distribution of CCDFs defined by the integrals in Eq. (7)?, and How to define and calculate quantities that relate the uncertainty characterized by the distribution of CCDFs to the uncertainty characterized by $(S_2, \mathcal{S}_2, \mu_2)$.

The preceding questions will be discussed in the context of recent performance assessments for reactor accident consequences and radioactive waste disposal. The applicability of various uncertainty and sensitivity analysis techniques will be considered and the analysis procedures selected for use will be described.

The Sensitivity of Models of Groundwater Flow to Conceptual Model Uncertainty and its Importance in Radionuclide Transport Problems

D. A. Zimmerman, GRAM, Inc., Albuquerque, NM, USA
Ghislain de Marsily, University of Paris, Paris, France
Steven Gorelick, Stanford University, Palo Alto, USA
M. G. Marietta and Carl Axness, Sandia National Laboratories, Albuquerque, NM, USA

In classical sensitivity analyses, the objective is to evaluate the influence of uncertain input parameters on the model output for the purpose of acertaining which are the more important parameters. In this study, we develop a novel application of classical sensitivity analysis procedures for the purpose of identifying which methods or modeling approaches are better suited for solving a problem which is plagued by conceptual model uncertainty. The interest of this approach is that it recognizes the importance of conceptual model uncertainties beyond model parameter uncertainties, and because it enables the relative importance of these two sources of uncertainty to be assessed.

The setting for this study is the Waste Isolation Pilot Plant (WIPP) site in southeastern New Mexico, USA, where disposal of radioactive wastes from defense programs of the U.S. Department of Energy (DOE) is being considered in a deep geological salt formation. Large uncertainties in the hydrogeologic flow regimes in the aquifer overlying the proposed repository lead to several plausible but conceptually very different models of important hydrogeologic properties in the aquifer in which the transport of radionuclides is of concern. Hence, the uncertainty in the spatial variability of the aquifer's log-transmissivity distribution can not be completely characterized via parameter uncertainty alone. A significant proportion of the uncertainty in the model output is due to the variation in the aquifer's characteristics as represented by different conceptual models of inferred hydrogeologic features. Thus, while different conceptual models do not have assigned values in the same way that model parameters range over different values, the sensitivity analysis nonetheless allows us to assess the importance of considering alternative sets of assumptions regarding the hydrogeology of the system.

Several state-of-the-art geostatistical inverse methods associated with these different conceptual models are currently being considered for possible use as performance-assessment tools as part of the effort to evaluate the potential of the WIPP site to comply with regulations governing the release of radionuclides into the environment from such facilities. In this exercise, we develop and utilize several "synthetic sites" (numerical analogs to the real site) to examine the effect that different conceptual model assumptions and parameter distributions of the mathematical model have on both the *accuracy* and the *precision* of the model predictions. Our objective is to evaluate the predictive capacity of different conceptual models once they have been calibrated to the sample data from the synthetic sites. Seven different conceptual models are compared. The presentation will emphasize the degree to

which the different conceptual models are able to cope with "synthetic sites" which do not necessarily meet the simplyfing assumptions of the conceptual models and will compare the robustness of these models.

SAMPLING METHODS AND SENSITIVITY ANALYSIS FOR LARGE PARAMETER SETS

T.H. Andres (andrest@wl.aecl.ca)
AECL Whiteshell Laboratories, Pinawa, Canada R0E 1L0

Many scientific modelling exercises produce a computer program to evaluate a scalar function $f(\mathbf{x})$, where $\mathbf{x} = (x_1, \ldots, x_n)$ is a vector of parameter values. (Without loss of generality, assume each x_i comes from the interval [0,1].) For example, in risk assessment studies, f may be a measure of environmental impact or harm, and the parameter vector $\mathbf{x}$ describes a possible state or series of states of a facility corresponding to a future scenario. In most studies, the expected value of f (denoted f_0) and the dependence of f on each of the parameters are of interest.

Often only a few of the parameters and groupings of parameters have significant impacts on f. When n is large (i.e., $n > 500$) it is difficult to find the few important parameters. Nevertheless, in (3) $n \sim 3300$ parameters were successfully screened for their impact on the output of a model of a deep geological waste disposal concept. This paper stems from that work. It describes an efficient sensitivity analysis (SA) procedure designed to elicit as much information as possible about the parameter dependencies of f based on function values at specific points.

1. Criteria for a Good Sensitivity Analysis Procedure

Formally, the purpose of an SA study is to characterize the variability of f as it is affected by variations of parameters in $\mathbf{x}$. Informally, the modeller's goal is to simplify his/her understanding of the model. The modeller wants to be able to explain an observed value of f by referring to values of a designated subset of the parameters.

The first step in reaching this goal is screening: i.e., to identify a parameter subset that controls most of the variability of f. This step is not always feasible. For example, if , and all x_i vary similarly, the function depends on all parameters equally, and no simplification is possible. A good SA procedure should work with "typical" applications. It should let the modeller know when it works and when it does not. In addition, it should:

- Reliably rank parameter effects.
- Produce repeatable results using the same procedure but different data sets.
- Minimize cost: the number of function evaluations needed should be much less than the number of parameters when n is large and few effects are important.
- Detect sensitivity across the entire domain of each parameter.
- Provide useful estimates of f_0, and of parameter influences.

2. Choosing Parameters for Sensitivity Analysis

The following variable types should be considered for parameters in an SA study, though only those in the first two categories are traditional parameters. When the number of parameters is already large, additional parameters do not complicate the study overmuch.

•Continuous parameters. Each domain (finite or infinite) should be transformed to the interval [0,1] for comparability. When the cumulative distribution function (cdf) $P_y(y)$ is known for a parameter y, it provides a suitable invertible transformation (3).
•Categorical variables that take qualitatively different discrete values.
•Constant parameters. Constants provide control variables. Any constant found to be important by screening indicates that the analysis has reached its resolution limits.
•Model controls (e.g., the number of time steps used in a simulation). These hidden variables can affect results. SA can estimate the magnitude of their influence.
•Artificial variables. Suppose $f(\boldsymbol{x})$ is the sum of several functions (e.g., pathways) g_j

(1)

where the b_j's are artificial variables. Each b_j normally takes the constant value 0.5 to leave f unchanged. In SA studies, b_j can vary from 0 to 1, acting like a valve that turns $g_j(\boldsymbol{x})$ off or on. Treated as parameters, the b_j's make it possible to assess the importance, not just of individual parameters, but of whole sections of a model.

3. Preparation of Sample Sets

Many options are available in setting up a sample set for screening analysis (3). The iterated fractional factorial design (IFFD) method used in (1) combines them all (3).

•Stratification. Balanced sampling from distinct levels (strata) allows the analyst to decompose output variance into two parts: that due to differences between levels, and that due to variation within levels. Latin hypercube sampling stratifies each parameter independently. Fractional factorial designs can balance sampling from discrete levels for two or three parameters.
•Discretization. By restricting a stratified sample to one value for each stratum, variation within parameter levels is eliminated. Some important variation may be missed, however.
•Orthogonalization. Orthogonal samples isolate the effects of individual parameters by avoiding inadvertent correlations with important parameters. Simple random and latin hypercube samples can be modified to reduce inadvertent rank correlations (3). Fractional factorial samples can be made orthogonal by design.
•Grouping. Each parameter in a group gets the same sequence of values in a subset of simulations. Suitable groupings can induce intended correlations of 1 and -1 between parameters, which can help to distinguish parameter effects.
•Folding. Pair every simulation with parameter values $(x_1, ..., x_n)$ with a simulation with parameter values $(1\text{-}x_1, ..., 1\text{-}x_n)$. The analyst can then distinguish between linear effects of individual parameters and effects of 2-way interactions.
•Replication. Important parameters exhibit self-reinforcing effects in most replicates. Unimportant parameters may appear significant in individual replicates, but spurious effects cancel out. Replicates give ad hoc estimates of statistical variation.

4. Analysis of Results

The formulation above treats only one function $f(\boldsymbol{x})$, but it is more informative to analyze multiple independent output variables $f_i(\boldsymbol{x})$. There is an optimal number of output variables: fewer would yield less information, and more would cost too much to analyze.

Saltelli et al. (4) assessed many SA techniques on two specific models and found comparable results for different methods. They showed, however, that rank analyses (where the result of the k'th simulation is replaced by its rank) are more repeatable than those based on $f_j(x)$ values. Other transformations of output variables can also improve analysis results. Linear models should be analyzed on a linear scale, whereas multiplicative models yield more information when log $f_j(x)$ is analyzed. Power transformations give intermediate results.

5. Evaluation of Results

To evaluate a parameter screening (i.e., a ranking of parameters in diminishing order of their influence), two types of studies are recommended:

- To evaluate the effects of discretization, repeat the simulations with parameters not discretized (not mapped to discrete values). Compare simulations in pairs, with and without discretization; apply SA to differences in $f(x)$ between pairs to identify parameters whose discretization has the greatest impact.
- To evaluate the effectiveness of a screening, run three sets of simulations. In the first set, vary all parameters using simple random sampling. In the second, use the values from the first set for the important parameters, but hold all other parameters constant at their central value. In the third, hold the important parameters constantä at a central value, and reuse the values from the first set for the others. In a successful screening, the variance of results in the second set should almost equal that in the first; the variance in the third set should be negligible in comparison.

References

(1) Goodwin, B.W., D.B. McConnell, T.H. Andres, W.C. Hajas, D.M. LeNeveu, T.W. Melnyk, G.R. Sherman, M.E. Stephens, J.G. Szekely, P.C. Bera, C.M. Cosgrove, K.D. Dougan, S.B. Keeling, C.I. Kitson, B.C. Kummen, S.E. Oliver, K. Witzke, L. Wojciechowski and A.G. Wikjord. 1994. The Disposal of Canada's Nuclear Fuel Waste: Postclosure Assessment of a Reference System. Atomic Energy of Canada Report AECL-10717 (COG-93-7).

(2) Stephens, M.E., B.W. Goodwin and T.H. Andres. 1993. Deriving parameter probability density functions. Reliability Engineering and System Safety 42 271-291.

(3) Andres, T.H. 1987. Statistical Sampling Strategies. Proceedings of an NEA Workshop on Uncertainty Analysis for Performance Assessments of Radioactive Waste Disposal Systems, held in Seattle, 1987 February 24-26.

(4) Andres, Terry H. and Wayne C. Hajas. 1993. Using Iterated Fractional Factorial Design to Screen Parameters in Sensitivity Analysis of a Probabilistic Risk Assessment Model. Proceedings of the Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, held in Karlsruhe, 1993 April 19-23, 2 328-337.

(5) Iman, Ronald L. and W.J. Conover. 1982. A Distribution-Free Approach to Inducing Rank Correlation among Input Variables. Commun. Statist.-Simula. Computa. 11(3) 311-334.

(6) Saltelli, A., T.H. Andres and T.Homma. 1993. Sensitivity analysis of model output—An investigation of new techniques. Computational Statistics & Data Analysis 15 211-238.

Statistical Approaches for the Exploratory Modeling of Large Complex Models

by

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USA

INTRODUCTION

Highly detailed computer simulations have become a common tool for a wide variety of research and analysis activities, including studies of global climate, economic activity, and military effectiveness. Our focus is on the use of large military combat models to support research; however, most of the ideas and methods are germane to the use of large models in other analytic applications.

Combat is extremely complex, and hence combat models can be too. It is not uncommon for combat models to contain many hundreds of thousands of lines of computer code using several megabytes of input data. The mathematical model implemented in the computer code effectively maps input variables X=(X1, ...,Xn) to output measures Y=(Y1, ...,Ym). We will denote this as Y=h(X)+e, where h represents the model and e represents the distribution of variation due to random numbers generated by the model. In practice, the dimension of X may be in the thousands, while h is highly nonlinear and discontinuous--and sometimes even chaotic, as brutally demonstrated by Dewar, Gillogly, and Juncosa, (1991). The computer codes are sufficiently complex that it often takes many hours to produce a single output. As a consequence, it is rare one can obtain more than perhaps a few hundred samples from the model. This challenging situation is further complicated by the fact that many events in combat models have to be characterized with some degree of randomness--that is, modeled using Monte Carlo methods. Typical examples include detection and attrition processes. This requires that the analyst characterize results statistically, rather than deterministically--which further burdens the sampling requirements.

As if the above challenges were not sufficient, combat models, unlike the engineering models used in CAD systems, can not be compared with actual outcomes. Indeed, many combat models are used to reason about hypothetical futuristic systems. In these cases there is typically uncertainty, or lack of knowledge, that implies there are many models and parameter settings that might plausibly represent the systems of interest. Thus, running a few best-estimate cases is a recipe for self deception. Instead, credible reasoning requires that conclusions be based on inferences about the entire ensemble of alternative plausible models and scenarios, as detailed in Bankes (1993). The problem of analysis thus focuses on the sampling strategy of how to select the limited number of computer experiments from the huge number that might potentially be relevant in order to inform the question of interest.

This paper introduces a novel approach to understanding how simulation models, that may not reliably make quantitative predictions about the behavior of the natural system, and for which a complete sensitivity analysis is impossible, can still be used to support credible reasoning. This approach formalizes individual computational experiments as samples from a space or ensemble of alternative model realizations. Strategies for reasoning under uncertainty dictate a wider range of potential objectives for the exploration of model space than is classically considered. Relative to this formalism, we devise resource constrained sampling strategies that combine adaptive search for models with special characteristics with a triage approach to designing series of experiments utilizing mixtures of high resolution, screening, massive group screening, and Monte Carlo designs. This method is illustrated on a large combat model in a study of the effectiveness of information systems.

REASONING WITH LARGE NONPREDICTIVE MODELS

Despite all the difficulties above and uncertainties inherent in combat models, decisions must be made, which may involve billions of dollars and put lives at risk. Those in the communities that use high resolution simulations are faced with a dilemma. While they may be convinced that such models can provide important insights that support decision-making under uncertainty, the computational unfeasibility of conducting a thorough sensitivity analysis as classically understood, exposes them to significant danger of being misled by anomalous model results. The normal approach is to ignore this risk and treat the model as predictive with known reasonable sensitivities. Hence, due to processing constraints, the studies vary only a few of the, believed a priori, key variables--while holding the remaining thousands of variables constant; however, inferences gleaned from the model are typically assumed to extend off of the tiny hyperplane in model space examined.

An alternative approach, detailed in Bankes (1992) and Dewar et al., (1995) is to consider the credibility of the combination of human argument and supporting computational experiments. Credible patterns of argument to support decision-making under uncertainty can allow constellations of computational experiments to be informative, even though the models used cannot be considered to make credible predictions of the behavior of the system of interest. Thus, instead of viewing models as prediction engines, we view computational experiments as infrastructure to support reasoning. Such experiments deduce implications of the posits required to specify a particular experiment. Reasoning strategies outside of the models themselves provide the context that make the outcomes of the modeling experiments salient. Thus, we reason over an ensemble of carefully designed plausible cases, rather than, employ a few samples presumed to be predictive.

A variety of reasoning strategies can be used to reason credibly in spite of large uncertainties. For example, risk aversion can motivate a search for plausible worst case scenarios, and the subsequent discovery of plausible disasters can credibly assist the design of policy even though none of the models employed can be demonstrated to predict system behavior. Similarly, the use of a fortiori arguments can be used to discount the importance of some uncertainties, and result in an interest in extreme rather than best estimate cases. As a general feature, such reasoning

strategies are typically concerned with characterizing the qualitative behavior of plausible system models rather than developing quantitative predictions of system behavior.

DESIGNING EXPERIMENTS FROM THE ENSEMBLE OF ALTERNATIVES

Given that one will reason over an ensemble of plausible runs constrained by time and budget considerations, the goal of the experimental design is to select those cases which will provide the most leverage in our research strategy. In detail, the DOE includes selecting the specific model(s) and variable settings. The key is to link the information needed from the multitude of variables, supplemented with expert reasoning, to the information obtainable from various experimental designs. It is assumed here that there are many more variables than samples available, as is almost always the case with large combat models. It is also assumed that in the regions of model space of interest some expertise exists and the number of causal factors and interactions is manageable (if this is not true the model is too unstable to draw general conclusions from inside of the constraints on computation).

Different designs are required for different classes of information. As part of a design triage, we propose that the analysts partition the model's variables into classes depending on their expertise and the information needed from varying the variables. In general, there are those variables and interactions from which we are primarily interested in or we think are causal; there are variables we believe are not significant, but must screen for, and there are variables which we only want to assess general model stability with respect to. Each of these classes implies a different class of design. The designs trade-off the information obtainable with the samples required to obtain it. For these different classes of information required we recommend combinations of specific designs, ranging from high resolution factorial, to fractional factorial, to main effects screening, to massive group screening, to random perturbations. Guidance on how to implement the combinations within imposed constraints is also provided.

This design philosophy allows a more comprehensive understanding of the model space within constraints. Typically, the success of this approach relies heavily on the ability of the experts to perform the design triage.

EXAMPLE

An example which shows how exploratory modeling and the design triage discussed above can support decision-making will be provided in the full paper. Here exploratory runs are made to determine plausible outcomes within the large land combat model JANUS in support of developing tactics techniques and procedures to better utilize new equipment.

CONCLUDING REMARKS

To avoid being fooled by our own models we need to rethink how we use very large non-predictive models to help decision-making. Rather than relying on a few model predictions, we need to support reasoning through carefully selected plausible model

outcomes. Combinations of different classes of experimental designs should be aggressively used to select the specific runs, or plausible cases, which efficiently support decision-making in an uncertain environment. A complex design strategy, which allows researchers variable levels of resolution, facilitates the estimation of effects and various level interactions on the key variables, while simultaneously screening other factors and assessing general model stability.

SENSITIVITY ANALYSIS OF DYNAMIC BUILDINGS ENERGY SIMULATION MODELS USING GROUP SCREENING AND SAMPLING METHODS.

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Introduction

For many years now, model output reliability and validity became topics of prime importance in many fields [1], however, only too few works have already been undertaken for buildings energy models.

Within the context of collaborations with Electricité de France (F) and the Building Research Establishment (UK), the LETIEF laboratory has developed and tested tools for modelling errors diagnosis by comparing model output with experimental data [2]. We are now interested in identifying the parameters to which model predictions are most sensitive (sensitivity analysis) on the one hand, and in quantifying the propagation of the uncertainty of these prevailing parameters (uncertainty analysis) on the other hand.

This paper deals with the application of screening methods to the sensitivity analysis of a building thermal model developed on CLIM2000, a software designed at the Research Centre of Electricité de France at Les Renardières

The objective of this work is to exhibit the most influent parameters among the 390 used in the model, and then to show that output uncertainty can be accurately derived using the uncertainty of these prominent parameters.

The building under analysis

The modelled building is the E.T.N.A. test cells, a real-size experimental building, including two identical symmetrical cells, surrounded by fixed temperature volumes. Extensive data acquisition and processing capabilities are also provided.

During the experiment the south wall was submitted to actual climate conditions. Thermal guards were maintained at constant temperature. The heating was switched on during the last 3 days of the 6 days experiment.

The building components thermo-physical properties and geometrical dimensions constitute model parameters. The nominal values used for these parameters came from the literature. The relative error related to the previous was taken as 5%.

We analyse the model prediction of the indoor air temperature.

The techniques used for sensitivity analysis

Although classical screening methods are efficient for models with a small number of parameters, they become unsuitable when this number reaches several hundreds. Consequently, we apply the group screening method [3], which allows to consider a great number of parameters. This method partitions the parameters into groups and test whether these groups have a significant effect. Then, all parameters of the non significant groups are eliminated and new groups are formed with the remaining parameters. The procedure continues, until remaining parameters are few enough that

we can apply classical designs.

The uncertainty analysis is then undertaken on the most influent parameters by *Monte Carlo* methods by using SPOP/PREP statistical processor [4]. The confidence interval thus derived is then compared with the one computed when using all the parameters.

The parameters screening

At each stage of the screening investigations, we apply Placket and Burman designs [5], which allow to assess the main effects of the different groups or factors, by use of a small number of simulations (k+1 simulations for k factors). Such designs suppose additive parameters effects, but since for the used parameters variations, interactions are likely to be small, the previous hypothesis holds. The factors are then sorted with the Lenth method [6].

After 4 stages (i.e. 136 simulations and 13,6h cpu time), 22 factors were selected from the initial 390. Although the parameter sorting depends on time, the 22 most influent factors are all related to the north wall, the floor and the south wall glazing.

- The north wall:

This wall is made of two plasterboards separated by an air gap. The parameters selected are the thermal conductivities, the thicknesses and the surfaces of the inner plasterboard and of the air gap. The two surface exchange coefficients are also influent.

The investigation of these effects during the 6-days simulation shows that conductivities, surfaces and surface exchange coefficients act in the same direction, while thickness acts in an opposite way. These behaviours were expected regarding conduction and convection flow equations.

On another hand, the magnitudes of these effects increase when the heater is switched on. This can be explained by the fact that the heat flow over the north wall raises as indoor air temperature raises while north guard temperature remains controlled at 10°C.

- The floor:

The two first components of the floor (from inside to outside) are concrete slab and insulator. The six parameters found important are the internal surface exchange coefficient, the concrete thickness, surface, specific heat, and specific volume and the insulation conductivity.

The exchange coefficient effect becomes significant when the heater is switched on. Then it decreases rapidly while the heater is still on. This can be explained by the fact that the inner air temperature raises before the floor surface temperature inducing a large heat convective flow. When the surface temperature raises, the flow diminishes and hence reduces this coefficient effect.

The insulation thermal conductivity is influent only during the heating period whereas the concrete parameters effects vary with both solar radiation and heating excitations

- The Glazing :

The 8 influent factors are the glazing surface, conductivity , the diffuse flow absorption and transmission coefficients, azimuth and tilt angle. The direct flow transmission coefficients for 40° and 50° incidence angle are also influent.

The glazing surface and tilt angle have large effects. Unlike the tilt angle and optical glazing parameters effects, the surface and the conductivity effects are sensitive to heater operation.

The Model output uncertainty band

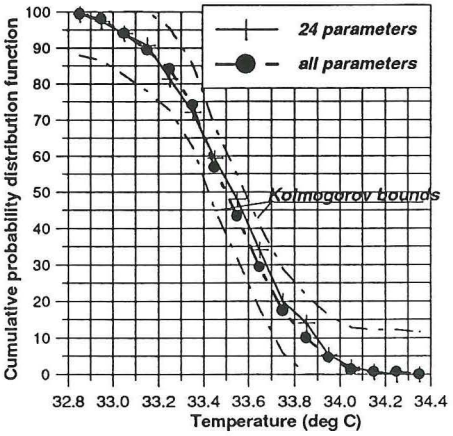

Figure 1 : model output distribution functions.

In order to verify that the model output global uncertainty is adequately described by the uncertainties of the chosen parameters, we compare two distribution functions : the first is the one computed by a *Monte Carlo* sampling of all 390 model parameters and the second in the one computed with the 22 parameters.

Figure 1 indicates the distribution functions obtained with 150 runs for model prediction at the end of the simulation. The Kolmogorov bounds are also drawn for the all parameters case. This figure shows the good agreement between the two functions : model output global uncertainty is accurately described by the uncertainties of the 22 parameters.

Conclusion

The application of group screening methods to the sensitivity analysis of building thermal models has demonstrated their efficiency to help sorting the parameters effects with a small simulation cost when the model involves a large set of parameters.

During the configuration analysed, the effects derived was found related to the magnitude of the heat exchanges between building components.

BIBLIOGRAPHY

[1] R.L.IMAN, J.C.HELTON : An investigation of uncertainty and sensitivity analysis techniques for computer models, Risk analysis, 1988.

[2] N.RAMDANI : Validation Expérimentale et Analyse de signàux : Développement d'une méthodologie de comparaison modèle /mesures en thermique du bâtiment, Doctorat thesis, Paris XII, 94.

[3] J.P.C. KLEIJNEN : Statistical tools for simulation practionners, Marcel Dekker, New York, 1987.

[4] A.SALTELLI, T.HOMMA : Statistical PRE Processor and Statistical POst Processor, Program description and User guides, 1992.

[5] P.D.HAALAND, Experimental design in biotechnology, Marcel Dekker, N.Y. 1990

[6] R.V.LENTH : Quick and easy analysis of unreplicated factorials, Technometrics, Nov. 1989, Vol.31, N°4

The determination of maximum entropy distributions given fixed rank correlation, and numerical approximations for use in sensitivity analyses

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When parameter uncertainty is being modeled by a probability distribution one immediately incurs the curse of dimensionality - for example, 20 parameters in the model imply that (in principle) a probability distribution in 20 dimensions has to be specified. Because of this problem it is necessary to find and use simpler models without losing modeling effectiveness. In this paper we investigate a joint probability distribution that can be used to model a partially unknown distribution.

We consider the case of two random variables X and Y for which only marginal distributions and a rank correlation coefficient are known. We propose to model the joint distribution in question by that joint distribution which has maximal entropy (or equivalently, minimal information) among all candidate distributions.

This principle has been applied in a number of practical situations, for example in projects for the European Space Agency and the chemical company DSM, where probability distributions with maximal entropy have been used in the analysis of the propagation of uncertainty of model parameters in models trying to assess the risks of spacecraft and chemical plants.

The relative information of X with respect to Z, for continuous r.v.'s with densities $f_X(x)$, $f_Z(y)$ is given by

$$I(f_X|f_Z) = \int_{\mathcal{Z}} \log(\frac{f_X(\xi)}{f_Z(\xi)})\ f_X(\xi)d\xi\ . \tag{1}$$

(we assume that if $z \in \mathcal{Z}$ then $f_Z(z) > 0$).

Suppose now that we wish to model a joint distribution for (X, Y) for which we only have partial information, for example the marginals F_X, F_Y, and the rank correlation $\rho_r(X, Y)$. We choose as model the distribution having minimal relative information with respect to the uniform density on the unit square among all distributions which satisfy the given information.

For notational convenience we consider continuous bivariate distributions with density $f_{X,Y}(x, y)$ supported on the shifted unit square $A = (-\frac{1}{2}, \frac{1}{2}] \times (-\frac{1}{2}, \frac{1}{2}]$, having uniform marginals. Let $\mathcal{F}_\rho$ be the subclass of all distributions with uniform marginals and a correlation ρ, $-1 \leq \rho \leq 1$.

The distribution with density $f_{X,Y} \in \mathcal{F}_\rho$ that has minimal relative information $I(f_{X,Y}|u)$ among all distributions in $\mathcal{F}_\rho$ with respect to the uniform distribution u, is a solution of the following optimization problem.

$$\begin{aligned}
&\textit{minimize} && \int_A f_{X,Y}(x,y) \log(\, f_{X,Y}(x,y)\,)\, dxdy \\
&\textit{subject to} && \int_{-\frac{1}{2}}^{\frac{1}{2}} f_{X,Y}(x,y)\, dx = 1 \qquad \forall y \in (-\frac{1}{2}, \frac{1}{2}]\ , \\
& && \int_{-\frac{1}{2}}^{\frac{1}{2}} f_{X,Y}(x,y)\, dy = 1 \qquad \forall x \in (-\frac{1}{2}, \frac{1}{2}] \qquad (2) \\
& \int_A xy f_{X,Y}(x,y)\, dxdy = \rho\sigma^2\ , && f_{X,Y}(x,y) \geq 0\ .
\end{aligned}$$

We stress that this problem is not a standard convex optimisation problem as there are effectively an uncountable number of constraints. The problem of entropy maximisation under a finite number of constraints has been much studied in the literature.

The main result is

Theorem 1 *The solution $f_{X,Y}(x, y)$ of (??) equals*

$$f_{X,Y}(x, y) = \kappa(x, \theta)\kappa(y, \theta)e^{\theta xy} \tag{3}$$

where the coefficients $\beta_{m,i}$ of the Taylor series expansion

$$\kappa(x, \theta) = \sum_{m=0}^{\infty} \sum_{i=0}^{m} \beta_{m,i} x^{2i} \theta^{2m} \tag{4}$$

are given by the recursive relation (??)-(??)

$$\beta_{0,0} = 1 \tag{5}$$

$$\beta_{m,i} = -\frac{1}{(2i)!}\sum_{k=0}^{m-i}\left(\sum_{j=0}^{k}\beta_{k,j}\frac{(\frac{1}{2})^{2i+2j}}{2i+2j+1}\right) \quad \text{for } i=1,2,\ldots,m, \text{ and} \tag{6}$$

$$\begin{aligned}\beta_{m,0} = & -\sum_{k=1}^{m-1}\left(\sum_{j=0}^{k}\beta_{k,j}\frac{(\frac{1}{2})^{2j}}{2j+1}\right)+ \\ & \frac{1}{2}\sum_{s=0}^{m}\sum_{k=\max(0,s-m+1)}^{\min(s,m-1)}\left\{\frac{1}{((2m-2s)!)^2}\left(\sum_{j=0}^{k}\beta_{k,j}\frac{(\frac{1}{2})^{2m-2s+2j}}{2m-2s+2j+1}\right)\right. \\ & \left.\left(\sum_{j=0}^{s-k}\beta_{s-k,j}\frac{(\frac{1}{2})^{2m-2s+2j}}{2m-2s+2j+1}\right)\right\}.\end{aligned} \tag{7}$$

The relation between θ and $\rho(X,Y)$ is given by $\rho(\theta) = 12\sum_{n=0}^{\infty} b_n\theta^{2n+1}$,and the coefficients b_n of this series are given by the following expression in the $\beta_{k,i}$.

$$\begin{aligned}b_n = & \sum_{s=0}^{n}\frac{\left(\frac{1}{2}\right)^{2s+3}}{2s+3}\sum_{k=0}^{s}\left\{\frac{1}{(2s-2k+1)!}\sum_{m=0}^{n-s}\right. \\ & \left.\left\{\beta_{m+k,k}\sum_{l=0}^{n-s-m}\frac{\beta_{n-s-m,l}\left(\frac{1}{2}\right)^{2l+2s-2k}}{2l+2+2s-2k}\right\}\right\}.\end{aligned} \tag{8}$$

We stress the fact that, as we have a power series expansion for the density $f_{X,Y}$, it is straightforward to derive expressions for conditional distributions, conditional expectations, etc.. We illustrate this in this paper by the derivation of the relation between θ and ρ.

Since, even with the analytic expression for the maximum entropy distribution, it is difficult to simulate, an alternative algorithm for simulation has been developed. We show that the maximum entropy distributions can be well approximated by a mixture of diagonal band distributions (a simple family of joint distributions) where the mixtures are specified in terms of beta distributions. This enables us to characterise the one parameter family

of maximum entropy distributions in terms to a single function mapping the correlation to the beta parameter, and enables relatively speedy simulation for sensitivity analyses.

We would like to thank Roger Cooke, Isaac Meilijson, Michael Keane and Jos van Kan for the many discussion with us about this topic.

Sensitivity Analysis, Uncertainty Analysis, and Validation: a Survey of Statistical Techniques and Case Studies

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This paper gives a introductory survey of the techniques of sensitivity and uncertainty analyses, together with their application in the validation and optimization of simulation models.

Further, this paper proposes to distinguish four phases in a simulation study, namely
(i) screening,
(ii) sensitivity or 'what if' analysis,
(iii) uncertainty or risk analysis, and
(iv) optimization of the simulated system.

Phase (i): Screening

In the screening or pilot phase the modelers are searching for the important inputs (parameters, factors) among the many (for example, 281) conceivably important inputs. Classic experimental designs may require too much computer time, when the simulation study is still in its early phase with its many inputs.

Bettonvil and Kleijnen (1991) present a screening technique, called *sequential bifurcation*. They proceed sequentially (or stage-wise) and split up (or bifurcate) the aggregated inputs, as the experiment proceeds; at the end the important individual inputs are identified and their effects are estimated.

They applied their technique to a model for the greenhouse effect of carbon dioxide (CO_2) and other gases. This model, is a deterministic simulation model (set of non-linear difference equations). It was developed at the Dutch 'National Institute of Public Health and Environmental Protection' (abbreviated in Dutch to RIVM). Bettonvil and Kleijnen study only a part of a large RIVM model that is called 'IMAGE'. This part has 281 inputs. Bettonvil and Kleijnen found the 15 most important inputs after only 144 runs. It is remarkable that the statistical technique identified some inputs that were originally thought to be unimportant by the policy analysts.

Phase (ii): Sensitivity analysis

From the viewpoint of the users (clients, management, government) the important model inputs should be split into two types, namely inputs that are under the decision makers' *control* versus *environmental* inputs that (by definition) are not controllable.

Specifically, users want to ask *what if* questions (scenario analysis): what happens if controllable inputs are changed? Sensitivity analysis is defined in this paper as the systematic investigation of the reaction of model outputs to *extreme* values of the model inputs and to drastic changes of the model structure. For example, how does the average waiting time in a queueing model of (say) a supermarket change when the customer arrival rate doubles; what if the priority rule (a qualitative factor) changes from first-in-first-out (FIFO) to small-jobs-first (express

lanes)? So this analysis examines global, not local (marginal) sensitivities.

Further on, controllable inputs can be optimized; see phase (iv). Environmental inputs are examined in phase (iii).

For phase (ii), this paper proposes *regression (meta)models* to approximate the input/output behavior of the simulation model. This regression analysis gives better results if the simulation experiment is well designed. Practitioners often change one factor at a time. This design, however, gives less accurate estimators of the factors' (main) effects; moreover, this design can *not* estimate interactions among inputs. Better designs are provided by the classic statistical *Design Of Experiments* (DOE); examples are fractional factorials (of resolution 3, 4, and 5), such as 2^{k-p} designs.

Furthermore, regression analysis and DOE can be used to *validate* simulation models that lack input/output data. Models and submodels (modules) with *unobservable* inputs and outputs can be subjected to sensitivity analysis, in order to determine whether the model's behavior agrees with the judgments of the experts (users and analysts). In case of observable inputs and outputs, it is also useful to apply sensitivity analysis.

An example is provided by a military case study, concerning the hunt for mines on the bottom of the sea. Model validity is of major interest to decision makers and other users of models.

Phase (iii): uncertainty analysis

Sensitivity analysis (see ii) may show that some inputs of the model are important; yet the precise values of these inputs may not be known. Obviously these inputs must be inputs that can not be controlled by the users: *environmental inputs*. Then risk or uncertainty analysis becomes relevant.

In *uncertainty analysis*, values of the model inputs are sampled from prespecified distributions, to quantify the consequences of the uncertainties in the model inputs, for the model outputs. So the input values range between the extreme values investigated in sensitivity analysis. The goal of uncertainty analysis is to quantify the *probability* of specific output values, whereas sensitivity analysis does not tell how likely a specific result is. The differences between sensitivity analysis and uncertainty analysis are further explored in this paper; sensitivity and risk analyses remain *controversial* topics.

Risk analysis is used in *business and economics*, such as investment analysis (what is the probability of a negative Net Present Value?). In the *natural sciences*, uncertainty analysis is also popular.

The techniques for risk analysis are *Monte Carlo* sampling, including variance reduction techniques such as *Latin hypercube sampling*, possibly combined with regression analysis.

Phase (iv): optimization

The *controllable inputs* should be steered -by the decision makers- into the right direction. For example, in the greenhouse case the governments should restrict emissions of the gases concerned; in queueing problems, management may add more servers (such as check-out lanes at a supermarket).

This paper proposes *Response Surface Methodology* (RSM), which is a heuristic sequential technique that combines DOE (especially 2^{k-p} and central composite designs), regression analysis, and steepest-ascent hill-climbing.

An RSM case study is presented, concerning a steel tube manufacturer's

production planning system with 14 controllable inputs and several response types.

This paper is 'biased' by more than 25 years of experience with the technique of simulation, especially its statistical aspects and its application to problems in business, economics, environmental, agricultural, military, and computer systems. Both deterministic and stochastic (random) simulation models are discussed. The paper includes many references for further study.

Keywords. Validation, what if, regression analysis, least-squares, sensitivity analysis, uncertainty analysis, risk analysis, validation, designs of experiments, screening, Latin hypercube sampling, optimization, perturbation.

On Benefits and Drawbacks of Customary Sensitivity Measures

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Abstract

In the context of uncertainty quantification of results from computational models the term "Sensitivity Analysis" usually refers to the application of all methods, procedures and techniques which provide quantitative statements about the degree of impact of the individual uncertainty sources on the uncertainty of the final model results. Such statements are extremely useful since they can indicate where to place further efforts in order to reduce the uncertainty of model results as effectively as possible.

In principle such analysis can only be performed in a parametric and probabilistic form, i. e. all uncertainty sources must be represented by uncertain parameters and provided with appropriate probability distributions which quantify the uncertainty about the correct value of the parameter.

The results of a parameter sensitivity analysis should be quantitatively presented in form of parameter specific sensitivity measures, i. e. numbers which quantitatively indicate the impact of the uncertainty of a parameter on the uncertainty of a model output. On the basis of such sensitivity measures a parameter uncertainty importance ranking with respect to a given model output may be established. Obviously, for time dependent model results the resulting parameter ranking may also be time dependent.

It is worthwhile mentioning that in this context it is not meaningful to define a sensitivity measure deterministically as the partial derivative of the output quantity with respect to a parameter. For, the sensitivity measure should not indicate how numerically sensitive is a model result to a specific parameter, as partial derivatives do locally in parameter space, but rather how much the uncertainty of that parameter contributes to the uncertainty of the model result. (The term "Uncertainty Importance Analysis" would perhaps be more suggestive than the commonly used "Sensitivity Analysis".) Thus appropriate probabilistic sensitivity measures must be found which involve the probability distributions of the uncertain parameter as well as the deterministic relationship between model output and parameters given by the computational procedure.

Due to the very complex and time consuming computational models, particularly in performance assessments of waste disposal systems, it is clear that the desired sensitivity measures as well as uncertainty statements cannot be derived analytically but must be determined from samples, i. e. from appropriately selected parameter combinations and the results of the corresponding runs of the computer model.

Since the time and costs of computer code runs, particularly of waste disposal

performance assessment codes, are extremely high, it will not be possible to perform a separate parameter sampling and corresponding model runs for the purpose of sensitivity analysis. Therefore the same parameter sample as for uncertainty analysis with the corresponding model results must be used for sensitivity analysis, too. This is the usual starting point of a parameter sensitivity analysis.

Another problem in sensitivity analysis, rarely considered in the past, may arise in applications with dependent uncertain parameters.

It is often observed that in many applications in which the state of knowledge on parameter level is analyzed more thoroughly some parameters must be considered as dependent in the subjectivistic sense of probability interpretation.

The influence of parameter dependence on uncertainty results has long been recognized as important. Thus it will not be surprising that it can be of considerable impact on the results of sensitivity analyses, too.

The present contribution is therefore mainly concerned with the question how reliable are the sensitivity results obtained with the traditional sensitivity measures if the parameters are not independent.

The following correlation-regression related sensitivity measures are considered more closely: correlation coefficient (CC), partial correlation coefficient (PCC), standardized regression coefficient (SRC) and correlation ratio (CR). Several simple examples are presented.

To avoid inaccuracies due to possibly insufficient sample size the population versions of the traditional sensitivity measures are determined analytically.

For the simple linear models considered in the examples it can be seen that in the case of independent or weakly dependent uncertain parameters all traditional sensitivity measures can easily be interpreted and give the same results (except PCC).

In the case of stronger dependence between uncertain parameters the sensitivity results obtained by different sensitivity measures may differ substantially. Their interpretation may be questionable or even misleading. Thus the traditional sensitivity measures may not be appropriate.

Considering the "maximum increase in the multiple correlation R2" as measure of relative importance of the corresponding parameter, the resulting parameter ranking provides a well interpretable and mostly satisfactory sensitivity result in the general linear case. It may therefore be preferred to the traditional sensitivity measures. Moreover, it can also easily be estimated from samples.

Obviously, one can draw the same conclusions also for slightly nonlinear models, i. e. with high R2 value and with dependent parameters.

As usual, the transition from raw values to ranks may cover the monotone case, too.

However, examples will also show that in the general nonlinear and monotone case with small R2 value and dependent parameters the traditional sensitivity measures as well as the above "maximum increase in the multiple correlation R2" may not be appropriate. The straight forward generalisaiton considering the "maximum increase in the multiple correlation ratio" may possible be satisfactory theoretically but in real applications the computation of its sample version would require a sample size which can rarely be afforded.

Finally, it also will be discussed why the traditional sensitivity measures succeeded in providing useful parameter importance rankings in many practically relevant problems despite the difficulties explained above.

Applications of Sensitivity Analysis to Combustion Chemistry

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Sensitivity analysis has been widely used in chemical kinetics [1] and it has frequently been applied to combustion chemistry [2] for uncertainty analysis and for gaining insight into mechanisms. The main combustion simulation codes, including the programs of the
CHEMKIN [3] package or the RUN1DL package [4], all calculate local concentration sensitivities.

Most rate parameters in combustion are known with rather large errors. The uncertainties of reaction parameters are listed in collections of evaluated reactions. Combustion mechanisms usually include several hundred reaction parameters, but only some of them have to be known with high precision. These parameters are usually identified on the basis of local concentration sensitivities. Note, that global methods have not been used in combustion chemistry, while such methods have been applied widely to the uncertainty analysis of atmospheric chemical models.

The sensitivity matrix itself accounts for the change of a single variable as a result of the change of individual parameters. The simultaneous effect of parameter changes on the concentration of several species can studied as the sensitivity of objective functions. If the objective function is the sum of squares of deviations, then the sensitivity of this objective function, called overall sensitivity [5], is equal to the sum of squares of sensitivity coefficients. In the summation only the species present in the objective function have to be considered.

Principal component analysis (PCA) of the sensitivity matrix [5] also investigates the sensitivity of an objective function. PCA is applicable to the study of the effect of simultaneous parameter changes on several outputs of a model. This method is based on the eigenvalue-eigenvector decomposition of the cross-product of local sensitivity matrices.

Overall sensitivities and principal components can be used for uncertainty analysis. As an example, if the measured concentrations are considered in the objective function, PCA shows which parameters can be determined from the measurement. It can also indicate if only e.g. the ratio of two parameters can be determined from the measurement. Changing the initial concentrations, measurement times etc. allows an optimization of experiments.

Sensitivity analysis methods are well suited to the investigation and reduction of combustion mechanisms. Inspection of concentration sensitivities has the advantage over the study of reaction rates in that sensitivities also account for non-direct effects.

The traditional approach for the identification of rate limiting steps was finding an appropriate analytical expression for production rates. This method is not applicable in the case of large reaction mechanisms. It has been assumed, without justification, that the high sensitivity reactions are identical to the rate limiting steps. Recently it was shown [1] that identification of rate limiting steps on the basis of the time derivative of the concentration sensitivity matrix is in agreement with the classical definition and yet can be applied to mechanisms of any size.

While, in uncertainty studies the initial time of sensitivity calculations is always

identical to the initial time of simulations, in mechanism investigation sensitivity analysis can be applied to a narrow interval during the simulation. The features of a mechanism depend on the concentrations and change continuously during a simulation. By moving this observation window, changing features of a mechanism can be monitored. For example, PCA can be used to detect which are the QSSA species and the redundant reactions during the interval inspected.

The logical extreme of this concept is the study of mechanisms at a single time, i.e. at a fixed concentration vector. Dynamical sensitivities are not applicable here, but the sensitivity of reaction rates becomes a useful measure. The partial derivative matrix of production rates with respect to kinetic parameters is equal to the matrix normed reaction rate contributions [6]. The principal component analysis of this matrix reveals kinetic details of the mechanism and allows the detection of ineffective parameters and hence leads to the reduction of the mechanism.

The Jacobian of the kinetic ODE shows the sensitivity of reaction rates to the concentrations. This matrix can be used for finding redundant species in the mechanism [7] and for the calculation of the instantaneous error of QSSA species [8].

A program has been written for the KInetic aNALysis of Combustion mechanisms. This program, called KINALC, is a postprocessor to the simulation programs of the CHEMKIN package. It has been interfaced to the programs of the CHEMKIN package (SENKIN, PREMIX, PSR, SHOCK, and EQLIB) and also to the RUN1DL package.

KINALC carries out three types of analysis: processing concentration sensitivity analysis results, extracting information from reaction rates and stoichiometry, and providing kinetic information about the species.

KINALC can extract the important pieces of information from the sensitivity results dumped by the simulation programs. It can also calculate the sensitivity of objective functions, formed from the concentrations of several species. Principal component analysis of the concentration sensitivity matrix can be used for uncertainty analysis, parameter estimation, experimental design, and mechanism reduction. The program can also suggest a list of rate limiting steps.

Principal component analysis of the algebraic rate sensitivity matrix provides an effective method for mechanism reduction. The program also offers traditional ways for mechanism investigation and reduction, such as rate-of-production analysis and calculation of the fluxes of elements from species to species and the contribution of each reaction to these fluxes. The analysis of the Jacobian allows a reduction in the number of species and the estimation of the instantaneous error of QSSA species.

KINALC has been designed to be very user friendly. It accepts simple keyword and may provide a detailed explanation of the results. The program has a modular structure and can be easily extended by other methods for the analysis of reaction mechanisms and can be interfaced easily to other simulation programs. KINALC is available from the World Wide Web at address:

http://chem.leeds.ac.uk/Combustion/Combustion.html

References:

[1] T. Turanyi
Sensitivity analysis of complex kinetic systems:
Tools and applications

J.Mat.Chem., 5, 203-248(1990)

[2] A.S. Tomlin, T. Turanyi, M.J. Pilling
Mathematical tools for the construction, investigation and reduction of combustion mechanisms
in: `Oxidation kinetics and autoignition of hydrocarbons'
ed: M.J. Pilling, Elsevier, in press

[3] R.J. Kee, F.M. Rupley, J.A. Miller
CHEMKIN-II: A FORTRAN chemical kinetics package for the analysis of gas-phase chemical kinetics
SANDIA report No SAND89-8009B

[4] Rogg B
RUN1DL: A computer program for the simulation of one-dimensional chemically reacting flows
Report CUED/A-THERMO/TR39, Cambridge, 1991

[5] S. Vajda , P. Valko , T. Turanyi :
Principal component analysis of kinetic models
Int.J.Chem.Kinet., 17, 55-81(1985)

[6] T. Turanyi, T. Berces, S. Vajda
Reaction rate analysis of complex kinetic systems
Int.J.Chem.Kinet., 21, 83-99(1989)

[7] T. Turanyi
Reduction of large reaction mechanisms
New J. Chem.,14,795-803(1990)

[8] T. Turanyi, A.S. Tomlin, M.J. Pilling
On the error of the quasi-steady-state approximation
J.Phys.Chem.,97,163-172(1993)

SENSITIVITY ANALYSIS OF NONLINEAR MODELS USING SENSITIVITY INDICES

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Abstract

Assume that the model under investigation is described by a function $f(x)$ defined in the n-dimensional unit cube I^n, so that $x = (x_1, \ldots, x_n)$.

1.Decomposition of the model function

The representation of $f(x)$ as a sum

$$f(x) = f_0 + \widehat{\Sigma} f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) \qquad (1)$$

is called *decomposition into summands of different dimensions* if $f_0 = const$ and the integral of every summand over any of its variables is zero:

$$\int_0^1 f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) dx_{i_m} = 0 \quad \text{for} \quad 1 \le m \le s.$$

Here the sum $\widehat{\Sigma}$ contains all f_i, $1 \le i \le n$, all f_{ij}, $1 \le i < j \le n$, all f_{ijk}, $1 \le i < j < k \le n$, ... The last member is $f_{12\ldots n}$ and the total number of summands is $2^n - 1$.

It follows from the definition that

$$f_0 = \int_{I^n} f(x) dx$$

and all the summands in (1) are orthogonal: if $(i_1, \ldots, i_s) \not\equiv (j_1, \ldots, j_l)$ then

$$\int_{I^n} f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l} dx = 0.$$

Theorem 1. *For an integrable function $f(x)$ the decomposition (1) is unique.*

Thus (1) is a finite orthogonal decomposition of $f(x)$ that doesnot depend on any prescribed orthogonal system.

2.Sensitivity indices

Assume that $f(x)$ is square integrable. Then all the summands in (1) are square integrable also, and the values

$$D = \int_{I^n} f^2(x) dx - f_0^2 \quad \text{and} \quad D_{i_1,\ldots,i_s} = \int_{I^n} f^2_{i_1,\ldots,i_s} dx$$

are finite. We call them *variances* because if x were a random variable uniformly distributed (u.d.) in I^n then D and $D_{i_1,\ldots,i_s}$ would be variances of $f(x)$ and $f_{i_1\ldots i_s}(x_{i_1},\ldots,x_{i_s})$. Squaring (1) and integrating over I^n we obtain the equality

$$\widehat{\Sigma} D_{i_1\ldots i_s} = D.$$

Definition. The ratios $S_{i_1\ldots i_s} = D_{i_1\ldots i_s}/D$ are called *global sensitivity indices* (SI).

Clearly,

$$\widehat{\Sigma} S_{i_1\ldots i_s} = 1.$$

Let $y = (x_{k_1},\ldots,x_{k_m})$ be an arbitrary fixed subset of variables: $1 \le k_1 < \ldots < k_m \le n$, $1 \le m < n$. Denote by $\mathcal{K}$ the set of integers $(k_1,\ldots,k_m)$. Then we define $S(y)$ as the sum of all SI with $i_1,\ldots,i_s$ belonging to $\mathcal{K}$, and $S^{tot}(y)$ — as the sum of all SI with at least one of the $i_1,\ldots,i_s$ belonging to $\mathcal{K}$. Evidently,

$$0 \le S(y) \le S^{tot}(y) \le 1.$$

The extreme cases are the most informative: If $f(x)$ is piece-wise continuous then 1^0 $f(x)$ doesnot depend on y if and only if $S(y) = S^{tot}(y) = 0$; 2^0 $f(x)$ depends only on y if and only if $S(y) = S^{tot}(y) = 1$.

3.Fixing unessential variables

Let z be the set of variables complementary to y, so that $x \equiv (y,z)$. If $S^{tot}(z) \ll 1$ it may be possible to replace $f(x)$ by $f(y,z_0)$ with a fixed z_0.

Indeed, let us consider the approximation error

$$\delta(z_0) = \frac{1}{D}\int_{I^n}[f(x) - f(y,z_0)]^2 dx.$$

For an arbitrary z_0 we have $\delta(z_0) \ge S^{tot}(z)$. However the following theorem is true:

Theorem 2. *The Lebesgue measure of the set of all z_0 from I^{n-m} having the property*

$$\delta(z_0) < (1+\varepsilon^{-1})S^{tot}(z)$$

exceeds $1-\varepsilon$ (for arbitrary $\varepsilon > 0$).

4.Computing sensitivity indices

In [1], a Monte Carlo algorithm has been defined that allows a direct estimation of $S(y)$ and $S^{tot}(y)$, without computing the summands

in (1). Each Monte Carlo trial requires two independent random points u.d. in I^n, $x = (y, z)$ and $x' = (y', z')$, and three computations of the model function: $f(x), f(y, z')$ and $f(y', z)$. Numerical examples can be found in [2].

References

[1] Sobol' I. M., Sensitivity estimates for nonlinear mathematical models. Matem. Modelirovaniye, 1990, Vol. 2, N 1, 112 – 118 = MMCE, 1993, Vol. 1, N 4, 407 – 414.

[2] Saltelli A., Sobol' I. M., Sensitivity analysis for nonlinear mathematical models: numerical experience. Ibid, 1995 (to appear).

ON AN ALTERNATIVE GLOBAL SENSITIVITY ESTIMATOR

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Abstract

Consider a function $f(x)$, $x = (x_1, \ldots, x_n)$, defined in the n-dimensional unit cube: $0 \le x_1 \le 1, \ldots, 0 \le x_n \le 1$. Let $y = (x_{i_1}, \ldots, x_{i_s})$ be a fixed subset of variables; we assume that $1 \le s < n$ and $1 \le i_1 < \ldots < i_s \le n$.

In [1] for estimating the influence of y on $f(x)$ global sensitivity indices $S(y)$ and $S^{tot}(y)$ were considered. Always $0 \le S(y) \le S^{tot}(y) \le 1$. In general, $S(y) = S^{tot}(y) = 0$ if and only if $f(x)$ doesnot depend on y, $S(y) = S^{tot}(y) = 1$ if and only if $f(x)$ depends only on y.

For a linear function $f(x) = a_1 x_1 + \ldots + a_n x_n$ one can easily compute that

$$S(y) = S^{tot}(y) = (a_{i_1}^2 + \ldots + a_{i_s}^2)/(a_1^2 + \ldots + a_n^2).$$

Thus, both indices are proportional to the sum of squared partial derivatives of $f(x)$. And an alternative global sensitivity estimate $G(y)$ seems physically reasonable:

$$G(y) = \sum_{k=1}^{s} \int_0^1 \cdots \int_0^1 \left(\frac{\partial f}{\partial x_{i_k}}\right)^2 dx \Big/ \sum_{i=1}^{n} \int_0^1 \cdots \int_0^1 \left(\frac{\partial f}{\partial x_i}\right)^2 dx.$$

The new estimator is hardly suitable for numerical computations. But in several analytical examples we have noticed that

$$S(y) \le G(y) \le S^{tot}(y), \qquad (1)$$

and this is an extra argument in favour of the sensitivity indices $S(y)$ and $S^{tot}(y)$.

We have investigated (1) for functions $f(x)$ with separated variables.

1. Variables of one type.

Consider a function

$$f(x) = \prod_{i=1}^{n} \varphi(x_i).$$

If $\varphi(x)$ and $\varphi'(x)$ are square integrable then (1) holds for all y.

Outline of a proof. Denote

$$c = \int_0^1 \varphi(x)dx, \quad u = \int_0^1 \left[\frac{\varphi(x)}{c} - 1\right]^2 dx. \tag{2}$$

The decomposition of $f(x)$ into summands of different dimensions [1] is

$$f(x) = c^n + \hat{\Sigma}[\varphi(x_{i_1}) - c] \cdots [\varphi(x_{i_s}) - c]\, c^{n-s}.$$

The estimators:

$$S(y) = \frac{(1+u)^s - 1}{(1+u)^n - 1}, \quad S^{tot}(y) = S(y)\big(1+u\big)^{n-s}, \quad G(y) = \frac{s}{n}.$$

Both inequalities in (1) are equivaleut to the assertion that $[(1+u)^s - 1]/s$ increases when s is increased, and this can be verified easily.

2. Variables of two types.

Consider a more general function

$$f(x) = \prod_{i=1}^{m} \varphi(x_i) \prod_{j=m+1}^{n} \psi(x_j). \tag{3}$$

In addition to (2) denote

$$d = \int_0^1 \psi(x)dx, \quad v = \int_0^1 \left[\frac{\psi(x)}{d} - 1\right]^2 dx.$$

The relation between the two types of variables can be described by one parameter

$$\varkappa = \left[\int_0^1 (\psi')^2 dx \Big/ \int_0^1 \psi^2 dx\right] : \left[\int_0^1 (\varphi')^2 dx \Big/ \int_0^1 \varphi^2 dx\right].$$

If the subset of variables is $y = (x_1, \ldots x_m)$, $1 \le m < n$, and $\varphi(x), \varphi'(x), \psi(x), \psi'(x)$ are square integrable then (1) is equivalent to

$$\frac{h_m}{(1+v)^{n-m}} \le \frac{n-m}{m} \frac{\varkappa}{(1+v)^{n-m} - 1} \le 1 + h_m, \tag{4}$$

where $h_m = [(1+u)^m - 1]^{-1}$.

Outline of a proof. Inequalities (4) can be derived from (1) using formulas $G(y) = \left(1 + \dfrac{n-m}{m}\varkappa\right)^{-1}$ and $S(y) = \dfrac{(1+u)^m - 1}{(1+u)^m(1+v)^{n-m} - 1}$, $S^{tot}(y) = S(y)\big(1+v\big)^{n-m}$.

3. Essential and nonessential variables.

Assume that the variables $x_{m+1}, \ldots, x_n$ in (3) are nonessential. Then a requirement that v is small can be introduced and from (4) a simple sufficient condition can be derived: Inequalities (1) are true if $nv \ll 1$ and

$$h_m \le \frac{\varkappa}{mv} \le 1 + h_m. \tag{5}$$

Example.

Consider the function (3) with $\varphi = 5x^4$, $\psi = 1 + \varepsilon \sin 2\pi l x$, l - positive integer. Here $c = d = 1$, $u = 16/9$, $v = \varepsilon^2/2$, $\varkappa = (7/72)\pi^2 l^2 \varepsilon^2 (1 + \varepsilon^2/2)^{-1}$.

The indices $S(y)$ and $S^{tot}(y)$ do not depend on l and as $\varepsilon \to 0$ both $S(y) \to 1$ and $S^{tot}(y) \to 1$. However if $\varepsilon \to 0$ and $l\varepsilon \to \infty$ one can see that $\varkappa \to \infty$ and $G(y)$ becomes irrelevant: $G(y) \to 0$.

Let $n = 20$, $m = 10$, $\varepsilon = 0.01$. Then $nv = 0.001 \ll 1$ and $h_m = 3.6 \cdot 10^{-5}$; condition (5) roughly means that $0 < 0.19\, l^2 < 1$ and is fulfilled for $l = 1$ and $l = 2$ only.

In fact, $S(y) = 0.99950$, $S^{tot}(y) = 1.00000$ while for $l = 1, 2, 3$ respectively $G(y) = 0.99990,\ 0.99962,\ 0.99914$.

References

[1] Sobol' I. M., Sensitivity estimates for nonlinear mathematical models. Matem. Modelirovaniye, 1990, Vol. 2, N 1, 112 - 118 = MMCE, 1993, Vol. 1, N 4, 407 - 414.

Global sensitivity analysis in nuclear problems

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ABSTRACT

There are uncertainties in every step of a probabilistic safety assessment (PSA) of nuclear installations. With the application of PSA in decision making procedures, the estimation of uncertainty becomes a most important question. Sensitivity Analysis(SA) in PSA which complements Uncertainty Analysis (UA) assists in the identification of influential model parameters, thus indicating where research effort is mostly needed toward the reduction of risk.

The present paper deals with a new method of global sensitivity analysis of nonlinear models. This is based on a measure of importance to calculate the fractional contribution of the input parameters to the variance of the model prediction. Measures of importance in sensitivity analysis have been suggested by several authors, whose work is reviewed in this article. More emphasis is given to the developments of the Russian mathematician I. M. Sobol', whose work on sensitivity indices is the most general. His formalism is employed throughout this paper where conceptual and computational improvements of the method are presented. The computational novelty of this study is the introduction of the "total effect" parameter index. This provides a measure of the global effect of a parameter, including all the possible synergetic terms arising from the coupling of that parameter with all the others. Rank transformation of the data is also introduced in order to increase the reproducibility of the method.

In Institute of Nuclear Safety(INS/NUPEC) PREP and SPOP codes originally developed in JRC/EC has been introduced to perform UA/SA with these new methods in each part of PSA for nuclear reactors. These methods are applied to the estimation of containment failure frequencies in BWRs. The performance of the methods with a new sampling scheme, using Sobol' quasirandom sequence are discussed with the comparison to both crude Monte Carlo sampling and Latin Hypercube sampling.

On the use of rank transformation in sensitivity analysis

by
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Abstract

Rank transformations are frequently employed in numerical experiments involving a computational model, especially in the context of sensitivity and uncertainty analyses. Ranks can cope with nonlinear (albeit monotonic) input-output distributions, allowing the use of linear regression techniques. Rank transformed statistics are more robust, and provide a useful solution in the presence of long tailed input and output distributions (Saltelli and Homma, 1992).

Care must be employed when interpreting the results of such analyses, as any conclusion drawn for the "ranked" model does not translate easily to the original model. In the present note an heuristic approach is taken, exploring, by way of practical examples, the differences between the original and the ranked models. This is done employing sensitivity indices, whereby the total variance of the model output is decomposed into a sum of terms of increasing dimensionality. The sensitivity indices were developed by Sobol' (1990, 1993), and have conceptual similarities with the Fourier Amplitude Sensitivity Test (FAST). Both methods allow the total model variance D to be written as the sum of terms of different dimension. The sensitivity indices have much in common with the importance measure discussed by other investigators (for a review, see Homma's work elsewhere in this volume).

The function $f(\boldsymbol{x}) = f(x_1,...,x_n)$ under investigation is defined in the n-dimensional unit cube:

$$K^n = \{\boldsymbol{x} \mid 0 \le x_i \le 1;\ i=1,...,n\} \qquad (1$$

Under assumptions described in Sobol' (1990, 1993) it is possible to decompose $f(\boldsymbol{x})$ into summands of different dimensions, eg:

$$f(x_1,...,x_n) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum\sum_{1\le i\le j\le n} f_{ij}(x_i, x_j) + \ldots + f_{12...n}(x_i, x_j, \ldots x_n) \qquad (2$$

where f_0 is a constant. At this point the sensitivity index $S_{i_1...i_s}$ can be introduced:

$$S_{i_1...i_s} = \frac{D_{i_1...i_s}}{D} \qquad (3$$

where

$$D = \int_{K^n} f^2(\boldsymbol{x})\, d\boldsymbol{x} - f_0^2 \qquad (4$$

is the total variance of $f(\boldsymbol{x})$ and

$$D_{i_1...i_s} = \int_0^1 \ldots \int_0^1 f^2_{i_1...i_s}\, dx_{i_1} \ldots dx_{i_s} \qquad (5$$

where $f_{i_1...i_s}$ denote a generic term of the series development (2). As shown in Sobol' (1990, 1993):

$$D = \sum_{i=1}^{n} D_i + \sum\sum_{1\le i\le j\le n} D_{ij} + \ldots + D_{12...n} \qquad (6$$

A consequence of (6) is that:

$$\sum^{\#} S_{i_1 \ldots i_s} = 1 \qquad (7$$

where the $\sum^{\#}$ notation indicate sum over all the combinations of indices. $S_{i_1 \ldots i_s}$ can be considered as true global sensitivity estimates, as they give the fraction of the total variance of $f(\boldsymbol{x})$ which is due to any individual parameter or combination of parameters. The sensitivity indices $S_{i_1 \ldots i_s}$ can be applied to a large class of functions $f(\boldsymbol{x})$ due to the possibility of evaluating the multidimensional integrals above via Monte Carlo methods. This is detailed in Sobol', 1990, 1993. (see elsewhere in this book; see also Homma and Saltelli (1994) for some computational improvement). In the following we shall also make use of "total sensitivity indices S_{Ti}. These give the total effect of variable each X_i. Imagine a system with just three input variables; then for variable X_1:

$$S_{T1} = S_1 + S_{12} + S_{13+} S_{123} \qquad (8$$

S_{Ti} can be computed with just one Monte Carlo integral. Both $S_{i_1 \ldots i_s}$ and S_{Ti} can be computed on ranks as well, with a net gain in robustness (Saltelli et al., 1993; Homma and Saltelli, 1994). The new measures are indicated with the symbols $S^*_{i_1 \ldots i_s}$ and S^*_{Ti}. For the present work the Monte Carlo integrals are computed with large sample sizes, using Sobol' LP_τ sequences for the sampling (Sobol', 1967). Quasi random numbers are characterised by an enhanced convergence, ie the $N^{-1/2}$ stochastic convergence rate of the crude Monte Carlo can - in some cases and depending on the nature of the function under investigation - become as large as $N^{-1+\varepsilon}$ with an arbitrary small $\varepsilon>0$ (see the work of Sobol', elsewhere in this book).

The plan of the present work is to use the difference between $S_{i_1 \ldots i_s}$ and $S^*_{i_1 \ldots i_s}$ (or their estimates) as a measure of the differences between f and f^*, where the latter represents the function which is obtained when both the input and the output values are replaced by their ranks. We show that the main effect of the rank transformation is to increase the relative weight of the first order terms, representing the linear effects, at the expense of the (synergistic) higher order ones. For the purpose of this abstract results are presented for a single test function of three indices i,j,k:

$$f_{ijk} = \sum_{i'=0}^{i} \frac{(ax)^{i'}}{i'!} + \sum_{j'=0}^{j} \frac{(by)^{j'}}{j'!} + \sum_{k'=0}^{k} \frac{(cxy)^{k'}}{k'!} \qquad (9$$

where a,b,c are arbitrary constants and x,y are independent variables uniformly distributed in [0,1]. The nonlinearity of f_{ijk} with respect to x,y and their cross product will depend upon the value of the indices i,j,k respectively. Also:

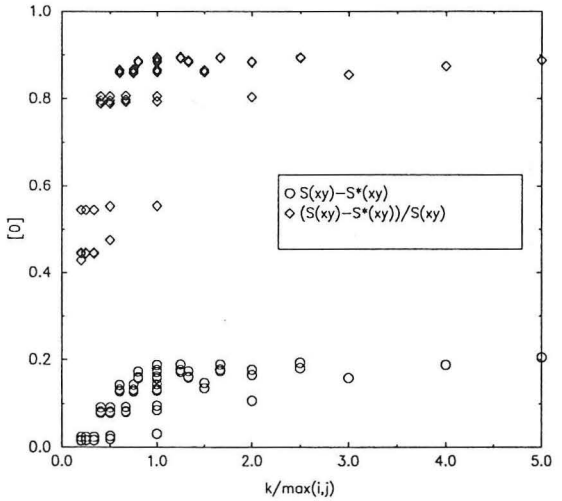
$$\lim_{\substack{i\to\infty \\ j\to\infty \\ k\to\infty}} f_{ijk} = e^{(ax)} + e^{(by)} + e^{(cxy)} \qquad (10$$

We can write the sensitivity indices of f_{ijk} and f^*_{ijk} as

$$1 = S_x + S_y + S_{xy} = S^*_x + S^*_y + S^*_{xy} \qquad (11$$

In the figure 1 we have plotted the values of $(\hat{S}_{xy} - \hat{S}^*_{xy})$ and of $\frac{(\hat{S}_{xy} - \hat{S}^*_{xy})}{\hat{S}_{xy}}$ versus the ratio $k/Max(i,j)$ for all the combinations of $i,j,k \in [1,5]$. For this Figure $a=b=1$; $c=3$, and a large LP_τ sample of base size $N=2^{15}$ was used. The figure shows that there is indeed a marked difference between f_{ijk} and f^*_{ijk}. The second order term, due to the coupling of x and y, can be completely overlooked (~ 90% error) by working on the rank transformed data. The error increases with the ratio of the importance of the second order term relative to the first order ones, ie with $k/Max(i,j)$. The other examples discussed in the present work suggest that those parameters which influence the output mostly by way of synergism may be overlooked in an analysis based on the ranks. This difficulty increases with the dimensionality of the problem, and may lead to the failure of a rank based sensitivity analysis.

Homma T., and Saltelli, A., 1994, Global sensitivity analysis of nonlinear models. Importance measures and Sobol'



sensitivity indices, European Commission, EUR report 16052EN, Luxembourg, 1994.

Saltelli, A., Andres T. H. and Homma, T., 1993, Sensitivity analysis of model output; An investigation of new techniques, Comp. Stat. and Data Analysis, 15, 211-238.

Saltelli, A., and Hjorth, J., 1995, Uncertainty and sensitivity analyses of dimethylsulphide OH-initiated oxidation kinetics, to appear in J. Atmos. Chem. (summer 1995).

Saltelli, A. and Homma, T., 1992, Sensitivity analysis for model output; Performance of black box techniques on three international benchmark exercises. Comp. Stat. and Data Analysis 13 (1), 73-94.

Sobol', I. M., 1967, On the distribution of points in a cube and the approximate evaluation of integrals, USSR Computational Mathematics and Mathematical Physics 7(4), 86-112.

Sobol', I. M, 1990 and 1993, Sensitivity estimates for nonlinear mathematical models, Matematicheskoe Modelirovanie, 1990, Vol. 2(1), 112-118 (in Russian), translated in Mathematical Modelling and Computational Experiments, 1(4) 407-414, 1993.

Sensitivity analysis for atmospheric chemistry models via automatic differentiation

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Keywords: Atmospheric chemistry, Automatic Differentiation.

1. Introduction.

The most common form of sensitivity studies with comprehensive atmospheric chemistry/transport models have been done using the so-called "brute force" method [1] , i.e., a number of input parameters are selected to be varied and the simulation results are then compared. This method becomes less viable as the model becomes more comprehensive.

A recently developed technique for sensitivity study is automatic differentiation technology. Automatic differentiation is implemented by precompilers that analyse the code written for evaluating a function of several variables. These pre compilers automatically add instructions needed to compute the required derivatives by properly handling quantities that are common to the function and its derivatives and by efficient use of available derivatives in a library. The resulting expanded code is then compiled with a standard compiler into an object code that can simultaneously evaluate derivatives and function values. This approach is superior to finite difference approximation of the derivatives because the numerical values of the computed derivatives are much more accurate and the computational effort is significantly lower (Griewank and Corliss, 1991; Griewank et al., 1993).

A promising new implementation developed at Argonne National Laboratory and Rice University over the last couple of years is the package ADIFOR (Automatic Differentiation in FORTRAN) (Bischof et al., 1992).

The chemistry kinetics problem may be formalised as follows. If $c_i(t)$ is the concentration of the i^{th} species, the kinetics of a chemical system is described as an initial value

[1] A variety of alternative techniques are also available including Green's function analysis (Cho et al., 1987), adjoint models and several variations of the direct decoupled methods (Dunker, 1984).

problem:

$$\begin{aligned} \frac{dc_i(t)}{dt} &= f(t, c(t), \beta_1, ..., \beta_m) = P(c(t)) - D(c(t)) \cdot c(t), \\ c_i(t_0) &= c_i^0, \qquad i = 1 \cdots n \end{aligned} \tag{1}$$

where β_j, $j = 1, ..., m$ are the parameters of the system (for example, reaction rate constants, etc), $P \in \Re^n$, $D \in \Re^{nxn}$, $D = diag(D_i)$ are the production and the destruction terms, respectively. By differentiating (1) with respect to the vector of parameters we obtain the variational equations:

$$\frac{d}{dt}\nabla c_i(t) \doteq \nabla P^i(c) - \nabla D^i(c) \cdot c_i - D^i \cdot \nabla c_i, \; i = 1, ..., n \tag{2}$$

2. Computational aspects with automatic differentiation.

The following were established during this study:

Result 1: By forward automatic differentiating a consistent (i.e., order one), prescribed step-size method for solving (1), one obtains a consistent method for solving the variational equation (2).

Result 2: The forward automatic differentiation applied to a fixed point scheme (e.g., the one resulting from solving the steady state equations for radicals) produces a fixed point scheme that solves a steady-state equation for sensitivities. This second scheme can be guaranteed to converge by taking some special precautions.

The above results show that direct differentiation of an existing code (for solving chemical kinetics) will produce a program able to correctly compute the sensitivity coefficients, provided the stated hypotheses are satisfied.

3. Direct method with automatically generated variational equations.

Our study shows that best results are obtained when generating (2) via automatic differentiation, then solving the variational system using an integrator of choice.

Looking at the variational equation (2) we remark that it is formulated in production - destruction form:

$$\begin{aligned} \frac{d}{dt}\nabla c_i(t) &\doteq \mathcal{P}^i(c) - \mathcal{D}^i \cdot \nabla c_i, \; i = 1, ..., n \text{ , where:} \\ \mathcal{P}^i(c) &\doteq \nabla P^i(c) - \nabla D^i(c) \cdot c_i, \; i = 1, ..., n \\ \left[\mathcal{D}^i(c)\right]_j &= D^i(c), \; i = 1, ..., n, \; j = 1, ..., m \end{aligned}$$

Hence, dedicated chemistry kinetics integrators can be employed, taking full advantage of their computational speed. In the study both methods (direct automatic differentiation of the existing algorithm and direct method with automatically generated variational equations) were tested; while the former is easier to apply, the latter is more accurate.

4. Application of automatic differentiation to a comprehensive atmospheric chemical mechanism.

The chemical mechanism used in this study is that presently used in the STEM-II regional scale transport/ chemistry/ removal model (Carmichael et. al., 1986). This mechanism consists of 86 chemical species and 178 gas phase reactions. To test the robustness of the above numerical algorithms, we have employed six different scenarios[2]. These conditions represent various chemical environments ranging from: low NO_x oceanic boundary layer regions (Marine); high NO_x continental boundary layer regions without (Land) and with isoprene (Bio); dry upper tropospheric regions; biomass burning plumes without (Plume 1) and with (Plume 2) reactive hydrocarbon species. ADIFOR 2.0 was used to calculate sensitivities of ozone with respect to initial conditions and reaction rate parameters.

5. Conclusions.

ADIFOR 2.0 has been successfully used in the sensitivity analysis of a comprehensive tropospheric chemistry model.

Automatic differentiation appears to be a valuable tool for sensitivity analysis of atmospheric chemistry models. In this paper we focussed solely on the chemical equations. However the method applies to the coupled transport/ chemistry problems as well. We are presently using this technique with the STEM-II model.

A valuable aspect of employing automatic differentiation for sensitivity analysis studies is that the atmospheric chemistry/ transport/ removal models are permanently subject to modifications and improvements. For routinely performing sensitivity analysis, one needs that, whenever a modification is performed in the model, the corresponding adjustment be made in the variational equations. Since the slightest mistake in the generation of variational equations could lead to useless results, one needs to thoroughly check for their correctness. Both the issues of

- easily generating the sensitivity equations and
- making sure they are error free

can be directly and successfully addressed by the use of automatic differentiation.

[2]These scenarios follow the IPCC (Intergovernmental Panel on Climate Change) photochemistry intercomparison.

IDENTIFICATION OF CRITICAL VARIABLES AND FUNCTIONS IN CHEMICAL SYSTEMS

by

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Sensitivity analysis of dynamical systems can provide a means for addressing (a) what is important in a model, and (b) how important the identified variables are. Often the first of these questions may be answered satisfactorily in a qualitative sense, while the latter subject is strictly quantitative and includes the statistical analysis of model performance in relation to input uncertainties. As a model is exercised at a nominal operating point in the parameter space, a local gradient sensitivity analysis is a powerful tool for identifying the key parameters and dependent variables in the model. However, when significant uncertainty exists in the input parameters, the linear sensitivities alone will not likely provide a reliable estimator of the output uncertainty in the model, in order to address question (b) above. The employment of global techniques are especially important in the latter context. The present paper will consider the use of local sensitivity analysis for identifying key parameters and variables in various problems of the chemical sciences. In addition, a guided Monte Carlo technique will be introduced to address statistical uncertainty issues.

A. IDENTIFICATION OF KEY VARIABLES.

Many problems in the chemical sciences can be categorized in a hierarchical sense, starting from the most intimate atomic scale and moving up to more macroscopic events, including such phenomena as combustion processes and atmospheric chemical dynamics.[1] A variety of physical length and time scales will transcend this hierarchy. Nevertheless, it must still be true that events at the atomic and molecular level, involving the shortest length and time scales, must have their impact on observable events at the macroscale. The linkage between these extremes poses interesting questions regarding which variables survive as being important, in the passage from one hierarchical level to another.

The utility of gradient-based sensitivity analysis to address these questions has been illustrated on a variety of chemical systems, involving molecular electronic[2], vibrational[3], and rotational motion[4] through the physical processes of intramolecular dynamics and molecular collisions. In turn, at the more macroscopic scale, chemical reactive kinetics, energy transfer, and transport processes also have been explored for their important information content with gradient-based techniques.[5] Two general classes of parameters need to be distinguished: those that are constants, and those that depend on the coordinates and/or time. In the former category, the sensitivities are partial derivatives of the output variables with respect to input parameters, while in the latter case, functional sensitivity densities are appropriate.

Finally, sensitivity analysis is most often utilized in the forward sense of analyzing how

the output depends on the input of a model. In turn, these same sensitivity coefficients and densities may be employed to develop efficient, stable inversion algorithms for extracting the underlying model parameters from laboratory data. In the chemical sciences, this application of sensitivity information has treated problems of inverse scattering and inverse spectroscopy.[6]

B. GUIDED MONTE CARLO ANALYSIS OF MODEL UNCERTAINTIES.

A common objective in chemical, or other types of modelling, is to assess the statistical quality of the output variables in relation to uncertainties in the input parameters. In the small uncertainty regime where linear sensitivity analysis is appropriate, the associated coefficients can be immediately employed to compute the output statistics from the input uncertainties. However, all too often, the model uncertainties will have an overall range that exceeds the linear regime. Various approaches to treating this problem have been and are being developed, as evident from much of this Symposium. A guided Monte Carlo technique may be especially effective in this context. Traditional Monte Carlo sampling of the input parameters and repeated execution of the model will eventually lead to the true output statistics. However, this process can be exceedingly expensive, when each model run is computationally intensive. This computational burden can be lessened by first observing that even if the input uncertainty distributions are broad, they are naturally centered around the nominal values of the input parameters. Thus, typical Monte Carlo runs will often correspond to samples that are in the linear or quasi-linear regime. These latter cases may be effectively treated by utilizing linear sensitivity coefficients for statistical mapping. In turn, the outlying extreme parameter variations are those best suited to Monte Carlo analysis. Thus, it is suggested to combine the two complementary approaches into an overall flexible guided Monte Carlo routine for statistical uncertainty analysis.[7]

In the guided Monte Carlo technique, the sensitivity coefficients serve two roles. First, they are used to estimate whether a given random sampling of the parameter space corresponds to a parameter set which is in the linear or nonlinear regime. If the linear regime is indicated, then the sensitivity coefficients are used to perform the mapping to the output. On the other hand, an identification of the nonlinear regime would lead to rerunning the model at the new point in the parameter space, and accumulation of that output to the statistics. Thus, an overall probability distribution of the output may be generated, involving a superposition of results from both the linear and nonlinear mapping regimes. Generally, the expectation is that the wings of the output distribution will be given by Monte Carlo runs, and the center, by sensitivity analysis. The guided Monte Carlo technique was explicitly developed in the context of chemical kinetic modelling, although it could just as well be applied to other areas.

In summary, it has been demonstrated that sensitivity analysis has a broad-based utility in the chemical sciences.

REFERENCES.

1. Systems Analysis at the Molecular Scale, H. Rabitz, Science, 246, 221 (1989).
2. On the Relation Between Electronic Structure and Molecular Dynamics, A. Lazarides and H. Rabitz, J. Chem. Phys., 93, 4192 (1990).

3. Mass Effects and Channel Coupling Sensitivity in Vibrational Energy Transfer, T.G. Kreutz, L. Eno, and H. Rabitz, J. Chem. Phys., 90, 1771 (1989).
4. Sensitivity Analysis of Mass Effects in Rotational Energy Transfer, T. Kreutz, L. Eno, and H. Rabitz, J. Chem. Phys., 88, 6322 (1988).
5. On the Role of Transport in the Combustion Kinetics of a Steady-State Premixed Laminar CO + H2 + O2 Flame, M. Mishra, R. Yetter, Y. Reuven, H. Rabitz, and M.D. Smooke, Int. J. Chem. Kinet., 26, 437 (1994).
6. Inversion of Experimental Data to Extract Intermolecular and Intramolecular Potentials, T-S. Ho and H. Rabitz, J. Phys. Chem., 97, 13447 (1993).
7. J. Shorter and H. Rabitz,to be published.

SENSITIVITY ANALYSIS USING LYAPUNOV EXPONENTS: APPLICATION TO CHEMICAL REACTORS

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1. INTRODUCTION

It is well known that, for certain values of the parameters in the mass and energy balance equations that represent the dynamic behaviour of chemical reactors, the system becomes very sensitive to the values of the initial conditions. Sensitivity to initial conditions is a well-known characteristic of chaotic phenomena. To study such systems, researchers have developed powerful methods of extracting physical quantities from theoretically or experimentally obtained signals (1). Between them, local Lyapunov exponents are the average exponential rates of divergence or convergence of nearby orbits in phase space (2). Since nearby orbits correspond to nearly identical states, exponential orbital divergence means that systems whose initial differences we may be not able to resolve will soon behave quite differently. This definition is, intuitively, related to temperature sensitivity concerning several input variables along the trajectory, corresponding to nominal operating conditions in the context of chemical reactor theory (3).

Local Lyapunov exponents were used in the definition of a generalised sensitivity criterion (4) in the context of single reactions in a batch reactor working under isoperibolic conditions: constant jacket temperature. In this work, this criterion is extended to cases where two consecutive or two parallel reactions occur simultaneously.

2. SENSITIVITY CALCULATION USING LOCAL LYAPUNOV EXPONENTS

Given a continuous dynamical system in an m-dimensional phase space, it is possible to monitor the evolution of an infinitesimal m-sphere of initial conditions. This m-sphere will become an m-ellipsoid due to the locally deforming nature of the flow. The jth one-dimensional local Lyapunov exponent, λ_j, is then defined (5) in terms of the length of the principal axes of the ellipsoid at time t, $p_j(t)$ as:

$$\lambda_j(t) = \frac{1}{t} \log_2 \frac{p_j(t)}{p_j(0)} \quad , j = 1,...,m \qquad (1)$$

The local Lyapunov exponent monitors the behaviour of two close neighbouring points in a direction of the phase space as a function of time. If the points expand away from each other, the Lyapunov exponent will be positive, if they converge, the exponent becomes negative, if the two points stay the same distance apart, the exponent stays

near zero. The sum of the local Lyapunov exponents gives the evolution of the volume of unitary hypersphere in the state space as follows:

$$vol(t) = vol(0)\, 2^{\mu} \tag{2}$$

where

$$\mu = \sum_{j} \lambda_j(t) \cdot t \tag{3}$$

As the volume increases, the trajectories of two neighbouring points in state space are separating i.e. the dynamic behaviour of the system undergoes a much larger deviation. For this reason, it is possible to define the sensitivity using Local Lyapunov exponents as follows:

$$s_{\phi} = \frac{\Delta \max_{t} 2^{\mu}}{\Delta \phi} \tag{4}$$

where ϕ is the parameter in relation to which we want to know the sensitivity of the system and μ is a function of the parameters of the system. In this frame criticality is defined as the value of ϕ for which Lyapunov sensitivity has the first extreme.

3. CASE STUDY: CONSECUTIVE AND PARALLEL REACTIONS

In this work we apply the sensitivity criterion using Lyapunov exponents to the case of an isoperibolic - constant jacket temperature- batch reactor where two reactions either consecutive or parallel occur simultaneously. The pertinent dimensionless equations representing mass and energy balances are:

Consecutive reactions $A \xrightarrow{1} B \xrightarrow{2} C$	Parallel reactions $A \xrightarrow{1} B$, $A \xrightarrow{2} C$
$\frac{du_A}{d\tau} = -f_1 u_A^{n_1}$	$\frac{du_A}{d\tau} = -f_1 u_A^{n_1} - \rho_2 f_2 u_A^{n_2}$
$\frac{du_B}{d\tau} = f_1 u_A^{n_1} - \rho_2 f_2 u_B^{n_2}$	$\frac{du_B}{d\tau} = f_1 u_A^{n_1}$
$\frac{dT}{d\tau} = \alpha f_1 u_A^{n_1} + \alpha \lambda_2 \rho_2 f_2 u_B^{n_2} - \beta(T-1)$	$\frac{dT}{d\tau} = \alpha f_1 u_A^{n_1} + \alpha \lambda_2 \rho_2 f_2 u_B^{n_2} - \beta(T-1)$
with initial conditions:	with initial conditions:
$u_A=1$, $u_B=u_B^i$, $T=T^i$ at $\tau=0$	$u_A=1$, $u_B=u_B^i$, $T=T^i$ at $\tau=0$

4. CONCLUSIONS

These reactions represent the situation in which one is dealing with a primary desired reaction which can be followed by an undesired exothermic secondary reaction. It is shown that the criterion based on Lyapunov exponents holds true also in these cases - see figs. 1 and 2 - and it can be used not only to identify critical parametic regions but also others in which the performance of the reactor is optimal.

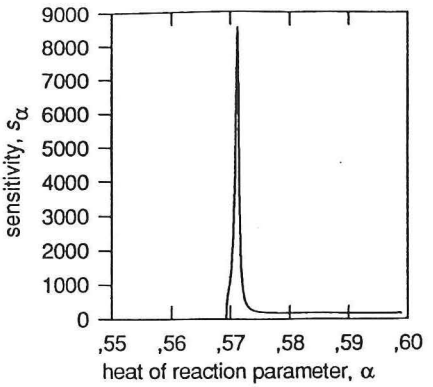

Figure 1. Sensitivity, see eq. (4), as a function of the heat of reaction parameter, α. Critical α at 0.5712. Value reported in (6) gives α_{crit}=0.5722.

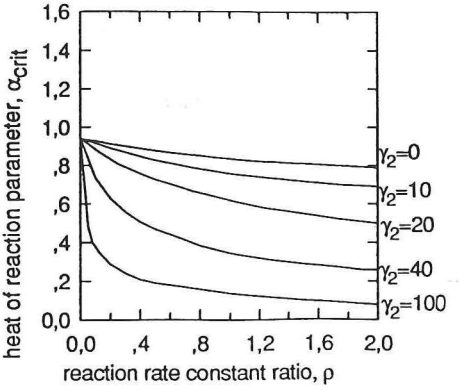

Figure 2. Effect of activation energy of the second reaction γ_2 in the case of two parallel reactions, see (6) for comparison.

NOTATION

- E activation energy
- f_i $\exp[\gamma_i (\overline{T}-1)/\overline{T}]$
- k reaction rate constant
- n reaction order
- S_v exchange surface area per unit volume, m^{-1}
- T dimensionless temperature, $\overline{T}/\overline{T}_a$
- $\overline{T}$ reacting mixture temperature, K
- $\overline{T}_a$ jacket temperature, K
- t time, s
- u dimensionless concentration, C/C_A^i
- U overall heat transfer coefficient, $W/m^2 K$

Greek symbols

- α dimensionless heat of reaction parameter, $(-\Delta H_1) C_A^i / \rho_f Cp \overline{T}_a$
- β dimensionless heat transfer parameter, $US_v/\rho_f Cp\, k_1(\overline{T}_a)C_A^{i\,(n_1-1)}$
- ΔH_i heat of i-th reaction, J/mol
- γ_i dimensionless activation energy, $E_i/R\,\overline{T}_a$
- λ_j heat of reaction ration, $\Delta H_j/\Delta H_1$
- ρ_f density, kg/m^3
- ρ_j reaction rate constant ratio, $C_A^{i(n_j-n_1)}\, k_j(\overline{T}_a)/k_1(\overline{T}_a)$
- τ dimensionless time, $k_1(\overline{T}_a)\, C_A^{i\,(n_1-1)}\, t$

REFERENCES

(1) Handley, J. W., Jaenisch, H. M., Bjork, C.A., Richardson, L. T. and Carruth, R. T., 1993, Chaos and Fractal Algorithms Applied to Signal Processing and Analysis. *Simulation* **60**, 261-279.
(2) Abarbanel, H. D., Brown, R., Sidorowich, J. J. and Tsimring, L. Sh., 1993, The analysis of observed chaotic data in physical systems. Rev. Mod. Phys. 65, 1331-1392.
(3) Bilous, O. and Amundson, N. R., 1956, Chemical reactor stability and sensitivity II. *A.I.Ch.E. J.* **2**, 117-126.
(4) Strozzi, F. and Zaldívar, J.M., 1994, A General Method for Assessing the Thermal Stability of Batch Chemical Reactors by Sensitivity Calculation based on Lyapunov Exponents, *Chem. Eng. Sci.* **49**, 2681-2688.
(5) Wolf A., Swift J.B., Swinne H.R., Vastan J.A., 1985, Determining Lyapunov exponents from a time series. *Physica* **16D**, 285-317.
(6) Morbidelli, M. and A. Varma, 1989, A generalised criterion for parametric sensitivity: Application to a pseudohomogeneous tubular reactor with consecutive or parallel reactions. *Chem. Eng. Sci.* **44**, 1675-1696.

ESTIMATING THE UNCERTAINTY OF A LAGRANGIAN PHOTOCHEMICAL AIR QUALITY SIMULATION MODEL (PAQSM) CAUSED BY INEXACT METEOROLOGICAL INPUT DATA

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Model description:

A Lagrangian photochemical air quality simulation model has been developed by the Institute of Meteorology and Physics in cooperation with the Austrian Research Center Seibersdorf. The model is based on 96 hours backward trajectories calculated from wind fields of the numerical weather prediction model operated by the European Centre for Medium Range Weather Forecasts (ECMWF) using the trajectory model FLEXTRA (1,2). The computation procedure used to get a representative transport level has been described in (3). For the last 12 hours of transport, local trajectories calculated from surface wind observations in Eastern Austria are blended with the synoptic scale trajectories to improve model performance, as pollutant concentrations highly depend on local transport patterns during the last few hours (4,5). Meteorological data along a trajectory are taken from ECMWF model analyses and from observations. Observation based surface and boundary layer data are computed using the OML Meteorological Preprocessor (6). The model consists of 8 vertical boxes, during the last 12 hours 3 horizontal boxes are simulated. Vertical diffusion is parameterized using Monin-Obukhov theory in the surface layer and K-profile closure in the stable boundary layer and unstable outer layer (7,8). Horizontal diffusion is parameterized during the last 12 hours of transport using constant exchange coefficients. Dry deposition of pollutants is simulated using (9). For the simulation of chemistry, the CBM-IV mechanism (10) has been implemented. Numerical integration is done using the QSSA method (11). European emissions are taken from the EMEP 1991 inventory, Austrian emissions are computed on a 5x5 km grid using the emission inventory of the Austrian Research Center Seibersdorf.

Tests of model performance:

Testing of model performance will be done by two means:

- Comparison of model results with ambient air quality measurements
- Sensitivity and uncertainty analysis

Preliminary comparisons of model results with routine O_3 and NO_x measurements had already been done. First results were very promising. Systematic multispecies comparisons, however, which are necessary for model validation, have not been done yet.

For sensitivity and uncertainty analysis, the following parameters of the model are of interest (12):

- Design parameters (simulation time, air parcel dimensions)
- Constitutive parameters (deposition velocity, exchange coefficients, chemical reaction rates)
- Model input data (trajectory position, meteorological input data, emissions)

Sensitivity analysis for meteorological model input:

Sensitivity analysis has been done for the following input data: temperature (TT), relative humidity (RH), boundary layer height (H_{pbl}), friction velocity (U*), surface sensible heat flux (F_h), precipitation (RR) and shortwave solar radiation (GR). As the base case scenario, calculations from July 1st, 1994 00 UTC to July 15th, 1994 00 UTC were done for receptor point Illmitz in Burgenland/Austria (16.769°E and 47.770°N). First, the relative sensitivity of chemical species C to meteorological input variable X was calculated:

$$S_{c,x} = \frac{|\overline{X}|}{|\overline{C}|} \left| \frac{\partial C}{\partial X} \right| \qquad (1)$$

Afterwards, the relative variances of meteorological input data within the air parcel had been taken to describe the uncertainty of the data:

$$R_x = \frac{1}{\overline{X}} \sigma_x \qquad (2)$$

Doing so, the total variance of the model output due to meteorological input can be calculated as follows:

$$\sigma^2 c = \sum_x S_{c,x}{}^2 R_x{}^2 \qquad (3)$$

Table 1 shows the results of sensitivity analyses for 4 chemical species in the first model box (0-30 m). In the case of O_3 and H_2O_2, the friction velocity U* turned out to be the most important parameter, because there is remarkable sensitivity combined with high data uncertainty. One important result of the analysis is that O_3 is one of the least sensitive species of the model, whereas other photooxidant and precursor concentrations are much more sensitive to input data variations and therefore more uncertain.

SPEC	PAR	|X/C| |∂C/∂X|	|1/X| sx	sc	SPEC	PAR	|X/C| |∂C/∂X|	|1/X| sx	sc
O_3	TT	8.60e+0	4.70e-3	1.98	NO	TT	6.70e+0	4.70e-3	0.0057
O_3	RH	3.30e-2	1.12e-1	0.18	NO	RH	1.19e-1	1.12e-1	0.0024
O_3	Hpbl	6.40e-2	3.37e-1	1.06	NO	Hpbl	5.45e-1	3.37e-1	0.0331
O_3	U*	2.00e-1	4.35e-1	4.26	NO	U*	2.65e-1	4.35e-1	0.0207
O_3	Fh	3.55e-2	4.93e-1	0.86	NO	Fh	1.12e-1	4.93e-1	0.0100
O_3	RR	2.00e-3	2.34e+0	0.23	NO	RR	6.30e-2	2.34e+0	0.0027
O_3	GR	2.65e-1	1.59e-1	2.06	NO	GR	1.43e-1	1.59e-1	0.0041

[O_3] = 49 • 10.6 ppb (21.7 %) **[NO] = 0.18 • 0.08 ppb (43.7 %)**

SPEC	PAR	|X/C| |∂C/∂X|	|1/X| sx	sc	SPEC	PAR	|X/C| |∂C/∂X|	|1/X| sx	sc
NO_2	TT	$6.90e^{+0}$	$4.70e^{-3}$	0.139	H_2O_2	TT	$9.65e^{+0}$	$4.70e^{-3}$	0.095
NO_2	RH	$2.20e^{-1}$	$1.12e^{-1}$	0.106	H_2O_2	RH	$9.05e^{-1}$	$1.12e^{-1}$	0.213
NO_2	Hpbl	$4.90e^{-1}$	$3.37e^{-1}$	0.710	H_2O_2	Hpbl	$2.10e^{-1}$	$3.37e^{-1}$	0.149
NO_2	U*	$1.03e^{-2}$	$4.35e^{-1}$	0.019	H_2O_2	U*	$4.00e^{-1}$	$4.35e^{-1}$	0.365
NO_2	Fh	$6.45e^{-2}$	$4.93e^{-1}$	0.137	H_2O_2	Fh	$6.45e^{-2}$	$4.93e^{-1}$	0.067
NO_2	RR	$1.25e^{-2}$	$2.34e^{+0}$	0.126	H_2O_2	RR	$1.20e^{-2}$	$2.34e^{+0}$	0.059
NO_2	GR	$4.25e^{-1}$	$1.59e^{-1}$	0.291	H_2O_2	GR	$7.90e^{-1}$	$1.59e^{-1}$	0.264

$[NO_2]$ = 4.3 • 1.5 ppb (35.5 %) **$[H_2O_2]$ = 2.1 • 1.2 ppb (57.7 %)**

Table 1: Sensitivity analysis for meteorological input data.

Monte Carlo simulation:

The Monte Carlo method is a technique widely used for data sampling. The data are varied using normal distributed random numbers. One base case scenario run and 9 Monte-Carlo scenario runs were done. The variances used for sampling are shown in table 2. The results of the Monte Carlo simulation are listed in table 3. As can be seen, Monte Carlo sampling shows smaller uncertainties than sensitivity analysis, with the exception of NO. However, both results show that the model output variation due to the variability and uncertainty of meteorological input data is within an acceptable range, especially as far as O_3 concentrations are concerned.

LON	LAT	TT	RH	Hpbl	U*	GR	Fh	RR	Kz	Ky	Vd	Sc
2.5/0.	2.5/0.	1.40	1.60	230.0	0.07	42.0	40.0	1.0	25.0	25.0	25.0	25.0

Table 2: Input data variances for Monte Carlo simulation. In case of trajectory position (LON,LAT), variance (given in degrees) is linearly reduced from beginning to end of trajectory. Kz and Ky are the vertical and horizontal exchange coefficients, vd is the deposition velocity and Sc the scavenging coefficient. For these four data, variances are given in % (s_X/X).

O_3	NO	NO_2	H_2O_2	PAN	CO
49.0 • 7.2	0.18 • 0.17	4.3 • 1.2	2.1 • 0.3	1.5 • 0.2	250.0 • 21.0

Table 3: Uncertainty of model output as computed in the Monte Carlo simulation. Mean values and standard deviations of species concentrations are tabulated in ppbv (confidence level 67%).

Literature:

1 Stohl A. and G. Wotawa (1994): FLEXTRA Version 1.0 Dokumentation. Institute for Meteorology and Geophysics, University of Vienna, September 1994.

2 Stohl A., Wotawa G., Seibert P. and H. Kromp-Kolb (1995): Interpolation Errors in Wind Fields as a Function of Spatial and Temporal Resolution and their Impact on Different Types of Kinematic Trajectories. Accepted for publication in *Journal of Applied Meteorology*.

3 Stohl A. and G. Wotawa (1995): A Method for Computing Single Trajectories Representing Boundary Layer Transport. Accepted for publication in *Atmospheric Environment*.

4 Wotawa G., Stohl A. and H. Kromp-Kolb (1993): Trajektorienanalyse für Wien und Niederösterreich während einer Ozonepisode am 31.7. 1992. Report to the Austrian Environmental Agency (Umweltbundesamt), Vienna

5 Stohl A. and H. Kromp-Kolb (1994): Analyse der Ozonsituation im Grossraum Wien. Österreichische Beiträge zu Meteorologie und Geophysik Heft 8.

6 Olesen H.R. and N. Brown (1988): The OML Meteorological Preprocessor. National Agency of Environmental Protection, Air Pullution Laboratory, DK-4000 Roskilde, Denmark.
7 Troen I.B. and L. Mahrt (1986): A simple Model of the Atmospheric Boundary Layer: Sensitivity to Surface Evaporation. *Boundary-Layer Meteorology* **37**, 129-148
8 Holtslag A.A.M., De Bruijn E.I.F. and H.-L. Pan (1990): A High Resolution Air Mass Transformation Model for Short-Range Weather Forecasting. *Monthly Weather Review* **118**, 1561-1575
9 Wesely M.L. (1989): Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models. *Atmospheric Environment* **23A**, 1293-1304
10 Gery M.W., Whitten G.Z., Killus J.P. and M.C. Dodge (1989): A Photochemical Kinetics Mechanism for Urban and Regional Scale Computer Modeling. *Journal of Geophysical Research* **94**, NO. D10, 12,925-12,956
11 Hesstvedt E., Hov O. and I.S.A. Isaksen (1978): Quasi Steady State Approximations in Air Pollution Modeling: Comparison of two Numerical Schemes for Oxidant Prediction. *International Journal of Chemical Kinetics* **10**, 971-994
12 US National Research Council (1991): Rethinking the Ozone Problem in Urban and Regional Air Pollution. National Academy Press, Washington, D.C.

THE EVEREST PROJECT : SENSITIVITY ANALYSIS OF GEOLOGICAL DISPOSAL SYSTEMS

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In the framework of the fourth R&D programme "Management and storage of radioactive waste" (1990-1994) of the European Commission (EC) the EVEREST project /1/ started in 1991. The main objective of EVEREST is the identification of the elements which strongly influence the performance of a geological disposal system. The conclusions of EVEREST are expected to contribute to the determination of research priorities in future R&D programmes. The EVEREST project is a collaboration between CEA-IPSN (Fontenay-aux-Roses, France), GRS (Cologne, Germany), ECN (Petten, the Netherlands) and SCK•CEN (Mol, Belgium). Three types of host formations (clay, salt and granite) and six sites are studied.

The EVEREST project can be considered as a complement to the earlier EC projects PAGIS /2/ and PACOMA /3/ which focused essentially on the development of a common European methodology for performance assessment of geological disposal systems. A typical characteristic of the developed approach is the application of as well deterministic as stochastic calculations in the assessment. Indeed it was found that the two approaches are strongly complementary and that each of them offers advantages that cannot be obtained with the other approach.

Within PAGIS and PACOMA a number of sensitivity studies have already been elaborated; these studies considered mainly sensitivity to the values of the model parameters. In EVEREST the concept uncertainty is considered in a broader perspective. Not only the uncertainties in the model parameters but also the uncertainties in the conceptual models and in the description of the scenarios are taken into account.

Most of the sensitivity analyses with respect to parameter values were carried out by making Monte Carlo simulations followed by sensitivity analysis mainly based on linear regression methods. Examples of effective sensitivity estimators are partial rank correlation coefficients and standardized regression coefficients. Non-parametric statistics like the Smirnov T statistic were applied to focus the sensitivity analysis on the small number of runs which yield the highest dose rates. For the parameter sampling as well random sampling as Latin Hypercube sampling were applied. In many cases Latin Hypercube

sampling was preferred because only a small number of runs, e.g. 40 runs for a problem with 25 independent variables, could be carried out due to the required computer times. A sampling scheme based on fractional factorial design has been applied for only one application where it was found that this approach is very effective for determining sensitivity estimators but it should not be recommended to evaluate the uncertainties in the calculated doses. Other sensitivity estimators have been used at GRS; these techniques are presented in another paper by Hofer /4/.

In the case of sensitivity studies on disposal in clay and granite small releases of radionuclides into the biosphere are calculated for each run of the Monte Carlo simulation. However a repository in salt provides a complete confinement of the disposed radionuclides as long as the geological salt barrier is intact. However after disruption of the salt layer the radionuclides are relatively fast released into the aquifer system. For some scenarios the sensitivity analyses can be complicated by the fact that only a small number of the runs in the simulation yield doses which are different from zero.

For the German salt site, a probabilistic sensitivity study using a very detailed near field model and a two-dimensional geosphere model has been performed. Nevertheless, especially the geosphere model was of a more generic type because several important effects occurring on the real site were not taken into account. Some problems occurred concerning the correct handling of a large number of runs which show a different numerical behaviour.

For some cases deterministic calculations were applied to evaluate sensitivities to parameter values. For an analysis of the sensitivity of the calculated water flow and transport to the values of the model parameters it is not evident how Monte Carlo simulations can be carried out because many combinations of parameter values will result in runs that are in conflict with, e.g., the observed piezometry. For the French clay and granite sites detailed two- and three-dimensional aquifer models are applied and the computer time needed for one calculation is considerable; therefore a deterministic sensitivity study based on a small number of calculations was preferred.

Detailed studies on uncertainties in conceptual models have been elaborated. These studies focused on the modelling of the behaviour of the host formations and the repository and on aquifer modelling. The potential impact of uncertainties in the migration mechanism in clay layers due to organic complexation was evaluated. For salt formations extensive sensitivity studies of the model for convergence and compaction of backfilled openings and of the modelling of the repository have been elaborated. In aquifer models considerable uncertainties occur which are due to uncertainties in the structure of the geology, i.e. thickness and extension of the various formations, faults and erosion channels, uncertainties in the boundary conditions and uncertainties in the parameter values because of the scarcity of the available observations and of spatial variability. The sensitivity analyses on conceptual model uncertainty carried out within EVEREST were mainly deterministic. Indeed large scale or three-dimensional aquifer models require extremely long computing times which makes that repetitive calculations, such as Monte Carlo simulations, are difficultly justifiable.

GRS has performed a stochastic study on conceptual model uncertainty by selecting randomly a geosphere model out of a set of eight possible models and by combining the selected model with randomly sampled parameter values.

An important aspect of uncertainty in the scenario description that received a lot of attention in EVEREST was the treatment of the expected evolution of the climate and its impact on the behaviour of the repository systems. Indeed forecasts of the climate for the next

100,000 years expect that a moderate glaciation will occur after about 25,000 years and a more severe one after about 70,000 years. These glaciations will strongly modify the water flow in the aquifer system because they cause changes in the amount of infiltrating water, in the aquifer condition, i.e. a phreatic aquifer might become confined by permafrost, and in the boundary conditions. The lowering of the sea level will strengthen the river erosion. At the very long-term the climatic changes will induce considerable uncertainties in the shallow components of the repository system, i.e. the aquifers and the biosphere. The sensitivity of the calculated doses to these uncertainties has been evaluated by performing a stochastic calculation in which the ranges of the parameter values enlarge with time, e.g. by increasing the standard deviation of the distribution.

Conclusions with respect to sensitivity analyses that can be drawn from the EVEREST exercise are that an approach based on Monte Carlo simulations and regression methods can be successfully applied. Some sites are now getting better characterized what makes that realistic modelling approaches including three-dimensional simulations are applied. However the considerable computer time needed for the elaboration of one single calculation causes problems for the application of Monte Carlo simulations. It appeàrs that efficient sampling strategies are needed. Another problem that arose during the elaboration of EVEREST was how to analyse problems were a large number of the runs yields zero outcome. Deterministic approaches were often preferred to make evaluations of conceptual model uncertainty in the geosphere models. Further developments are required on the systematic integration of uncertainties due to future climate changes in the performance assessment. A challenge for sensitivity analysis remain the evaluation of the sensitivity of the calculated dose rates to the combined uncertainties in the parameters values, the conceptual models and the scenarios descriptions.

REFERENCES

/1/ P. Escalier des Orres, J. Marivoet, J.M. Gomit, J. Prij and K.H. Martens
EVEREST : Evaluation of Elements Responsible for the Equivalent Doses Associated with the Final Storage of Radioactive Waste
EC, Luxembourg, report in preparation

/2/ N. Cadelli, G. Cottone, S. Orlowski, G. Bertozzi, F. Girardi and A. Saltelli
PAGIS : Performance Assessment of Geological Isolation Systems for Radioactive Waste
EC, Luxembourg, report EUR 11775 EN (1988)

/3/ PACOMA : Performance Assessment of the Geological Disposal of Medium-Level and Alpha-Waste
EC, Luxembourg, reports EUR 12993, 13042, 13143, 13178 and 13634 (1991)

/4/ E. Hofer and B. Krzykacz
On the benefits and drawbacks of customary sensitivity measures
(this conference)

Sensitivity of Radionuclide Release and Transport to Uncertainty and Variability in Properties of Deep Crystalline Rock. Examples from the SKI Repository Performance Assessment SITE-94

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Introduction

In Sweden the main alternative for disposal of spent nuclear fuel is repositories in deep crystalline rock. The potential safety of such repositories are analyzed through performance assessments that include model calculations of radionuclide release and transport via groundwater through the host rock. The input to such models depends upon properties both of the engineered barriers and on the properties of the geologic medium. In general these properties are both variable and uncertain, and their impact on the resulting releases can sometimes be strongly non-linear. Consequently, it is of high interest to explore model responses to potential uncertainties as such analyses provide insight into what degree of precision that is necessary in order to make precise enough predictions of repository safety. Such an uncertainty and sensitivity analysis has been part of a repository performance assessment research project, SITE-94 that is conducted by the Swedish Nuclear Power Inspectorate (SKI).

Treatment of uncertainty and variability

Site evaluation, with real site characterization data, is used to determine information of transport paths in the geosphere and to deliver information on geosphere interaction with the engineered barriers. Such evaluation involves development of alternative conceptual models, consistent with site data, both for the state of the disposal system immediately after repository closure and for the states after climatic changes. For each conceptual site model a suite of calculation cases, or variants have been developed. The basic methodology when constructing these variants was to parameterize scenario uncertainty, system uncertainty, conceptual model uncertainty and parameter uncertainty.

For a given conceptual model, the calculated parameter uncertainty and variability information is usually expressed in terms of intercorrelated ranges, distributions or sometimes as set of point values. In order to provide input to the radionuclide release and transport, that reflects parameter uncertainty and variability, this information has been abstracted into sets of single value parameter variants.

The hydrological transport properties in the geosphere can be characterized in terms of two parameter groups that control the radionuclide transport in the geosphere: "F-ratio" ($F = a*L/q$) and Peclet number ($Pe = q*L/(\theta*D_L)$), where a is the flow wetted surface, L is the transport distance, q is the Darcy velocity, θ is the flow porosity and D_L is the longitudinal pore water dispersion.

Each conceptual hydrology site model produces a range of values of these parameter groups reflecting the spatial variability of the hydrologic properties along different pathways. Figure 1 illustrates the results of two conceptual variants of a discrete fracture network hydrology site model. Each data point represents the

effective transport properties corresponding to the flow and transport paths from a single canister location. The encircled areas indicate the spatial variability associated with respective model variant.

It is necessary to reduce the number of parameter combinations further transferred to the radionuclide transport calculations, as they treat more than 30 nuclides and coupled near-field and far-field. The use of sensitivity analyses with simplified source terms for near-field and far-field separated, give aid in selecting calculation cases for the coupled analysis with the full source term.

Sensitivity analysis for the near-field

The sensitivity analysis for the near-field (waste-form, bentonite buffer and the rock surrounding the canister site) was performed with a simplified source term, consisting of 1 mole of a hypothetical, stable nuclide, released instantaneously from the fuel. In the analysis, hydrological parameters (e.g. near-field rock Darcy velocity and flow wetted surface) and chemical parameters (distribution coefficients for sorption and solubility limits) were varied.

The results from the sensitivity analysis show that the release rate is insensitive to model parameters above or below certain levels. The most obvious example is the Darcy velocity. For high Darcy velocity release from the near-field will be controlled by diffusion through the bentonite buffer, hence a further increase of Darcy velocity or changes of flow wetted surface will not affect the release rate. For medium and small Darcy velocities, increasing flow wetted surface in the near-field rock decrease the release rates. In these cases, changes in sorption distribution coefficients also have significant effect on the releases.

Sensitivity analysis for the far-field

The source term for the sensitivity analysis for far-field consisted of a delta function, i.e. an instantaneous release of 1 mole of a stable nuclide. The intention with these sensitivity calculations was to verify that the selected far-field parameter groups (F-ratio and Pe-number) can be used as hydrological performance measures for the radionuclide transport.

Different combinations of the F-ratio and Peclet number as well as different combinations of the individual hydrological input parameters a, q and D_L were analysed. The calculated peak release and time of occurrence were not affected by variations of the input parameters as long as the F-ratio and Peclet number were held constant. The peak release rates indicated a strong dependence on the F-ratio, with decreasing release rates with increasing F-ratio. The Peclet number affected the transport results to a lesser extent (high Peclet numbers give lower peak release rate).

Integrated near-field and far-field calculations

The full source term consists of the inventory of radionuclides, with different decay rates, some of them coupled in chains and with different release rates from the fuel. In the coupled calculations the output from the near-field calculations (time series of flux in Bq/year for each nuclide) is the input for the far-field calculations.

Sets of hydrological parameter values were selected from the "F-ratio/Peclet number space" (data points in Figure 1) to form calculation cases for the integrated analysis of radionuclide transport. Other uncertainties e.g. in geochemistry were treated with sets of parameter values. When selecting the parameter sets the results from the sensitivity analysis were used to reduce the number of calculation cases, and thereby

avoiding calculations that would most probably give the same result. When defining calculation cases for the integrated analysis correlations were taken into account to avoid combinations of near-field and far-field parameters that are inconsistent with data.

Results of integrated analysis

The integrated results comprised release of nuclides from the far-field. The integrated analysis of the radionuclide transport show that the total dose rate (i.e. summed over all nuclides) is totally dominated by release of I-129 in early times (10^3-10^5 years), and that the release of I-129 is almost insensitive to parameter variations. Which nuclide(s) that contributes most to the total release rate at later times (10^5-10^6 years) depends on the chemical and hydrological parameter values.

One of the main chemical uncertainties concerns the redox conditions in the near-field, and had a significant effect on releases. The high uncertainty and spatial variability of the estimated near-field Darcy velocity had a more limited effect. However, the relative importance of these uncertainties are nuclide specific.

Figure 2 illustrates the far-field release of Ra-226 for a reference near-field parameter set up, as a function of the far-field parameter uncertainty predicted by the hydrological site models. The far-field performance covers a very large span, from retarding most nuclides (high F-ratio) to releasing most of the input from the near-field (low F-ratio). These results underscore that spatial variability and model uncertainties have a significant impact on repository performance and on the relative importance of the near-field and far-field barriers.

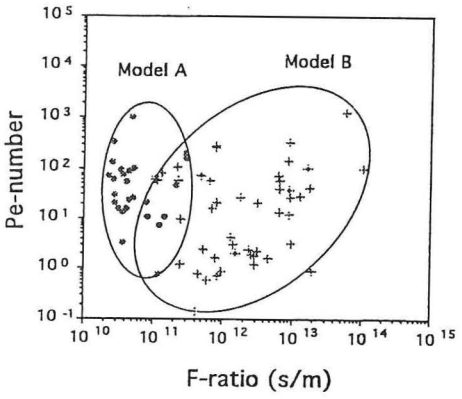

Figure 1. Far-field performance measure predicted by hydrological site models.

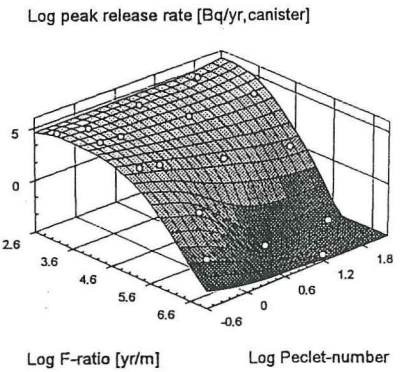

Figure 2. Sensitivity of far-field release as a function of hydrological parameter uncertainty.

Joint CEC/USNRC Post Processing for Uncertainty Analysis

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June 29, 1995

To estimate the risks and consequences of hypothetical nuclear accidents, the Commission of European Communities (CEC) and the United States Nuclear Regulatory Commission (USNRC) separately developed Probabilistic Accident Consequence Codes (PACC), COSYMA and MACCS, respectively. Since many code parameters are uncertain, these organisations decided jointly to establish a methodology and provide a base of information in order to perform uncertainty analysis on the calculations of PACC.

Since the available data is sparse and as both organisations wanted to allow for a diversity of viewpoints, formal expert judgement elicitation was used to quantify the uncertainty. The goal of expert judgement is to encode degree of beliefs into probability distributions. When subjective probability is recalled to its original meaning, it can only be used to measure an individual's degree of belief regarding outcomes of possible observations. Consequently, in this joint effort experts are only asked about physically observable quantities with which they are familiar. Variables which are physically observable and for which the expert has to provide information will be called *query* variables. Code parameters which uncertainty must be quantified in order to perform the uncertainty analysis are called *target* variables. Target variables may be query variables, but it can also arise that target variables are unsuitable as query variables, since they do not correspond to measurements which the experts can estimate.

Two examples from the joint project illustrate the distinction between query variables and target variables.

Example 1 The lateral plume spread σ_y is modelled in the codes as a power law

$$\sigma_y(x) = A_Y x^{B_Y} \tag{1}$$

where x represents the distance from the source and A_Y and B_Y are the target variables for the code. Experts have little feeling for the behaviour of A_Y and B_Y; indeed the physical dimension of A_Y must be $[\text{meters}]^{1-B_Y}$.

For this reason it was decided to elicit the experts over σ_y as this is a quantity which is measured repeatedly and with which the experts are familiar. Asking for the lateral plumespread means that the uncertainty analyst has to develop a method for determining a distribution on the code parameters A_Y and B_Y.

Example 2 The migration of radioactive material through various depths of soil is modelled using a so-called box model, see Figure 1. The target variables

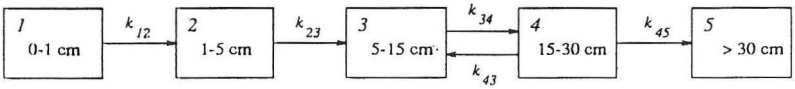

Figure 1: *Box-model of soil-migration*

for the code are transfer coefficients k_{ij}, which represent the proportion of material moved from box i to box j in a small time interval. Based on Figure 1, a set of first order differential equations can be constructed which, with the appropriate initial conditions, fully specifies the movement of the material between the boxes. The aim is to derive a distribution on all transfer coefficients. Transfer coefficients cannot be measured directly and therefore cannot be query variables. In this case the query variables were on times T_i when half of the mass of the deposited material has past beyond box i. From this information a distribution on the transfer coefficients has to be determined.

The determination of a distribution on the various target variables (A_Y, B_Y or transfer coefficients), given information on query variables (σ_y or T_i) is called post processing. For the first example a post processing technique has been developed, which is described in detail in [1], [2] and [3]. However this post processing technique is impractical in cases with the complexity comparable to that of the second example.

In this paper we will introduce a more powerful post processing technique. For purposes of illustration we describe the technique for the first example. Starting distributions are assigned to the target variables A_Y and B_Y. These distributions are propagated through the the power law (1) for distances $x_1, \ldots, x_n$ from the source. This will generate a joint distribution $F(\sigma_y(x_1), \ldots, \sigma_y(x_n))$. The expert has assessed the marginal distributions $G_1(\sigma_y(x_1)), \ldots, G_n(\sigma_y(x_n))$. We now find the distribution F^* having minimum information with respect to F and having marginals which agree with $G_1(\sigma(x_1)), \ldots, G_n(\sigma(x_n))$. The joint distribution (A_Y, B_Y) is extracted from the distribution F^*.

We will compare the two post-processing techniques for data from the first phase of the joint effort. The two post-processing schemes treat the information of

the expert in different ways. It is therefore interesting to investigate the sensitivity of the submodel outcomes with respect to the choice of post-processing technique.

References

[1] R.M. Cooke, L.H.J. Goossens, B.C.P. Kraan. *Methods for CEC/USNRC Accident Consequence Uncertainty Analysis of Dispersion and Deposition*, EUR-15856EN, Delft University of Technology, 1994.

[2] F.T. Harper, L.H.J. Goossens, R.M. Cooke, J.C. Helton, S.C. Hora, J.A. Jones, B.C.P. Kraan, C. Lui, M.D. McKay, L.A. Miller, J. Päsler-Sauer, M.L. Young. *Joint USNRC/CEC Consequence Uncertainty Study: Summary of Objectives, Approach, Application, and Results for the Dispersion and Deposition Uncertainty Assessments*, NUREG/CR-6244, EUR 15855, SAND94-1453. Sandia National Laboratories and Delft University of Technology, 1994.

[3] Cooke, R.M.. Parameter fitting for uncertain models: modelling uncertainty in small models. *Reliability Engineering & System Safety*, 44:89-102, 1994.

SENSITIVITY STUDIES OF AIR SCATTERED NEUTRON DOSE FROM PARTICLE ACCELERATORS

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Introduction

Increasing use of high current accelerators in densely populated locations for research and industrial purposes necessiates optimal design of overhead shields, thus requiring a sensitivity analysis of air scattered dose with respect to the effective parameters. We have carried out the senstivity analysis of the calculated air scattered neutron dose from a particle accelerator using the Response Surface Methodology(RSM). RSM has been chosen basically because this technique is widely used for sensitivity analysis of nuclear-safety related problems(1).In this approach a small subset of the system parameters after screening is first chosen for the study. Specific changes to be made in this data to address senstivity and uncertainity questions are thus derived from variety of experimental design theories(2,3). Initial sensitivity screening results(4) indicate that the overhead shield of the accelerator is the most sensitive parameter, followed by the high energy part of the source neutron spectra. The distance of the neutron source from the overhead sheild being the least significant has been removed from the parameter list. Source neutron spectra has been computed using two well known Nuclear Reaction models.The estimated distributions(high energy part) from the models PRECO-D2 and ALICE differ considerably necessiating quantification of the difference between the models. To overcome this difficulty we have binned the energy distribution in 5 groups,each group representing a parameter in the sensitivity analysis. Hence, in our study we have chosen six parameters, and performed sensitivity analysis with several experimental designs, a full 2^6 factorial design and other composite designs like Orthogonal Central Composite Design(OCCD), and a full 3^6 factorial design. We have found in this study that the contribution of the second order effects to the total variance is not significant and, hence OCCD and 3^6 are not necessary for the present analysis. Since ours is a computational experiment, measurement and observational errors are absent and the RSM, with the advantage of separating the statistical analysis from the modelling problem, detects the basic variability in the system. We have obtained sensitivity coefficients by expanding the response surface by a multivariate Taylor's series and incorporating the least square criterion of minimum error. We illustrate the successful use of the RSM in studying the behaviour of the sensitivity

coefficients of air scattered neutron dose at a distance from the accelerator with neutron emissions from 50 and 60 MeV α projectiles interacting with a thick Tantallum(Ta) target.

Method of Calculation

Let $D(r;t,E_j)$ be the neutron skyshine dose at a distance **r** meters from the accelerator, with **t** meters of overhead shield made of concrete, $\mathbf{E_j}$ being the energy distribution of the source neutrons(5) (j = 1...5).

We define

$$D(r;\vec{\alpha}) \equiv D(r;t,E_j) \tag{1}$$

where $\vec{\alpha} = (t, E_j)$ for j = 1...5 and reponse as

$$R_i = \frac{D(r;\vec{\alpha_i}) - D(r;\vec{\alpha_0})}{D(r;\vec{\alpha_0})} \tag{2}$$

for j = 1...5 where the index i is the number of design points chosen according to RSM and $\vec{\alpha_0}$ is the nominal vector around which 1% of perturbation is carried out. Using the overhead shield and five energy groups as parameters we have used a full six factor design (2^6). We define the response surface as

$$R^{rs} = \sum_{i=1}^{n} \beta_i a_i + \sum_{\substack{i=1 \\ j=1}}^{n} \beta_{ij} a_{ij} \tag{3}$$

where $a_1 = t, a_2 = E_1, a_3 = E_2, a_4 = E_3, a_5 = E_4, a_6 = E_5$, β_i = main effects, β_{ij} = interaction effects. We have neglected the higher order terms. We have obtained the sensitivity coefficients ie.,main effects and interaction effects of the parameter set by expanding the response surface by multivariate Taylor's series and incorporating the least square criterion of minimum error. In order to investigate the contribution of second order effects to the total variance we have studied a full 3^6 factorial design. Because of the prohibitive computational time required(3^6 = 729 treatment combinations) for such a calculation we have also considered an Orthogonal Central Composite Design(OCCD) which is more efficient and less time consuming. For q controllable variables OCCD can be constructed by taking $2q$ points with co-ordinates $(\pm\alpha,0,0,0,0,0),(0,\pm\alpha,0,0,0,0),\ldots,(0,0,0,0,0,\pm\alpha)$ and to these add the 2^q points $(\pm\beta,\pm\beta\ldots,\pm\beta)$. The constants α and β are chosen such that $\alpha/\beta = 2^{q/4}$. In our case we have taken β=1 and for q=6 controllable variables we get α=1.682. We have obtained sensitivity coefficients β_i, β_{ij} for a nominal vector $(2.0m, E_1, E_2, E_3, E_4, E_5)$ for 50 and 60 MeV α induced thick target neutron source distribution, both for experimentally measured and theoretically calculated using PRECO-D2 and ALICE.

Results and Discussions

The results indicate that the overhead shield is the most sensitive parameter then the high energy part of the source neutron distribution followed by the interaction term of the above two. Among the main effects for parameters (E_j, j=1 . . . 5) of the source neutron spectra, highest energy parameter of the source neutron distribution is most sensitive when compared with the other parameters. Also in case of interaction effects the interaction of overhead shield with the highest energy parameter is most sensitive when compared with the other interaction effects. These two cases demonstrate the ability of the RSM in quantifying the otherwise intutively known results. The sensitivity coefficients obtained with theoretical model PRECO-D2 has shown more variation than ALICE when compared with the data obtained using experimentally mesured source neutron distributions. This is due to the fact that both the theoretical models underpredict the source neutron spectra particularly the high energy portion.Hence our generated reponse which has quantified the inherent differences of the theoretical models when compared to experimental data, can be utilised in suitable modification to closely simulate the experimental situation.

References

1. Neil D.Cox, Nuclear Science and Engineering Vol.64,258(1977).

2. Box G.E.P, Draper N R, Empirical Model Building and Response surfaces, John Wiley and Sons, Inc., New York, USA(1987).

3. Kleingnin J.P.C, Statstical Techniques in Simulation - part II, Marcel Dekker,Inc., New York(1975).

4. Prabhakar Rao G. and Sarkar P.K, Journal of Testing and Evaluation (to be published in September 1995) ASTM,USA.

5. Prabhakar Rao G. and Sarkar P.K, Annals of Nuclear Energy Vol. 21 No.1(1994).

DIFFERENTIAL OPERATOR SAMPLING FOR SELF-OPTIMIZING MONTE CARLO SIMULATIONS

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The differential operator sampling technique has emerged as a very powerful tool in sensitivity analysis and has found typical applications in parameter estimation and parameter optimisation. Here we describe a new algorithm for constructing self-optimizing non-analog Monte Carlo simulations based on the differential operator sampling technique. Non-analog simulations are designed to reduce statistical errors (variances) associated with the scores (results) by introducing in the physical simulation certain artifacts. Effective implementation of such variance reducing schemes requires knowledge of optimal values of some parameters (biasing parameters), not known 'a priori'.

Based on the concept of differential operator sampling (1 to 7) it is now possible to differentiate with respect to those biasing parameters which aim at minimizing the variance in a non-analogue game. In this case we differentiate the second moment of the score with respect to the biasing parameters and extrapolate its dependence of the variance by a multi-variate Taylor series. This requires in most cases the determination of higher-order derivatives to obtain a reasonable approximation of the curve or surface containing the minimum. Our algorithm based on the multivariate Taylor expansion in terms of the first and higher order derivatives of natural logarithm of the second moment around the score in a non-analog Monte Carlo simulation, predicts the optimal biasing parameters corresponding to the minimum variance simulation. We have found that stochastic simulation processes incorporating our algorithm have the same transition kernels as those of the original simulation thus allowing the derivatives to be sampled from the same random walk. An iterative procedure incorporating such simulations and a feedback of information renders eventually the optimal biasing parameters. Numerical experiments have shown that the present technique finds the optima even in the cases of high statistical uncertainty, i.e., with a very few histories in a simulation. We illustrate the application in a slab transmission problem that utilizes the exponential transform as a variance reducing scheme in a non-analog Monte Carlo simulation.

As an illustrative example and a test we have considered the non-analog Monte Carlo random walk simulations of particle transmission through semi-infinite homogeneous slabs of different thicknesses (7 to 10). The simulations use the exponential transform as a variance reduction technique in a one-group isotropic scattering model. A plane parallel beam of particles is incident on one surface of the slab. Transmission through the other side of the slab is scored. The particles enter the slab with unit weight and after each collision their weight is modified by a multiplicative factor proportional to the survival probability: $p_s = \sigma_s / \sigma_t$ (with: σ_s and σ_t being the macroscopic scattering and total reaction cross sections). The other modifying factor is introduced by the biased transport kernel $T(x, x', \mu, \alpha) = \sigma_t^* \exp[-\sigma_t^*(x'-x)/|\mu|]/|\mu|$, where x and μ are space and direction coordinates, respectively, and $\sigma_t^* = \sigma_t (1 - \mu\alpha)$ is a biased reaction cross section modified by the direction cosine μ and the biasing parameter α, obeying the condition $0 \leqslant \alpha < 1$. We now calculate the first and higher-order derivatives of the second moment of the fluence (leaving the slab at d) with respect to α for a given value α_0, (which in most cases is assumed to be zero). For a Taylor expansion around $F(\alpha_0) = ln[M_2(\alpha)]$ we get

$$F(\alpha_0 + \Delta\alpha) = F(\alpha_0) + \Delta\alpha\frac{\partial}{\partial\alpha}F(\alpha_0) + \frac{(\Delta\alpha)^2}{2}\frac{\partial^2}{\partial\alpha^2}F(\alpha_0) + \frac{(\Delta\alpha)^3}{6}\frac{\partial^3}{\partial\alpha^3}F(\alpha_0) + \ldots.$$

To find the α-value for which the second moment (~variance) has a minimum we differentiate with respect to $\Delta\alpha$

$$\frac{\partial}{\partial(\Delta\alpha)}F(\alpha_0 + \Delta\alpha) = \frac{\partial}{\partial\alpha}F(\alpha_0) + (\Delta\alpha)\frac{\partial^2}{\partial\alpha^2}F(\alpha_0) + \frac{(\Delta\alpha)^2}{2}\frac{\partial^3}{\partial\alpha^3}F(\alpha_0) + \ldots.$$

Now, the value of $\Delta\alpha$ which gives the minimum variance, can be approximated by solving the equation

$$\frac{\partial}{\partial(\Delta\alpha)}F(\alpha_0 + \Delta\alpha) = 0$$

which yields

$$\Delta\alpha = \left\{-\frac{\partial^2}{\partial\alpha^2}F(\alpha_0) \pm \sqrt{\left(\frac{\partial^2}{\partial\alpha^2}F(\alpha_0)\right)^2 - 2\left(\frac{\partial^3}{\partial\alpha^3}F(\alpha_0)\frac{\partial}{\partial\alpha}F(\alpha_0)\right)}\right\} \cdot \left[\frac{\partial^3}{\partial\alpha^3}F(\alpha_0)\right]^{-1}$$

With the help of the above equations one can estimate the value of $\alpha+\Delta\alpha$ that will render a minimum-variance simulation.

In *Table I* we list results for transmissions through slabs of thickness 10 and 20 mean-free-paths (*mfp* in units of σ_t, respectively) and a scattering probability of 0.9. The results were obtained as averages over 200,000 histories for each value of the biasing parameter α. In each case we start out with an $\alpha_0 = 0$ and determine $\alpha+\Delta\alpha$. With this value the calculation is repeated until $\Delta\alpha < 0.01$. As is expected, the mean value for the fluence remains unchanged (allowing for statistical fluctuations), except for 20 mfp where the statistical fluctuations predominate. The second moment and the variance decreases with increasing α, reaches a minimum and then increases. The minimum in the variance is obtained for values α between 0.4 and 0.5 for $p_s = 0.9$ and close to 0.6 for $p_s = 0.8$ (not shown in the Table), irrespective of the thickness of the slab. These trends are in agreement with previous results (7) obtained for similar problems using deterministic estimates. It is also observed that overbiasing to a large extent leads to a higher variance compared to underbiasing. For example, $\alpha = 0.9$ produces a larger variance than $\alpha = 0$ (no biasing) for $p_s = 0.9$ for all slab thicknesses. The number of flights per history increases slightly with increasing α and then decreases. The trend remains the same for all slab thicknesses and scattering probabilities. This behaviour is expected as the exponential transform essentially decreases the modified cross section σ_t^*, in the directions of $\mu > 0$ (forward direction) and increases for $\mu < 0$ (backward direction).

It can be seen that the prediction at $\alpha = 0$ is very good for small thicknesses, deteriorating with increasing thickness, nevertheless pointing to the right direction and improving with α getting closer to its optimum value. The prediction is also poor when the system is overbsiased. This may be attributed to the fact that the sample variance is not a true indicator of the population variance (6, 8). Now, if we look at the values of F', F'' and F''', we can see that the values of F''' are large compared to those of F' and F''. This is particularly so, when the value of $(\alpha+\Delta\alpha)$ gives a poor estimate of the optimum. It is thus implied that for a more accurate prediction one has to consider more terms (i.e. higher order derivatives). Nevertheless, based on the algorithm described in this paper, one can design a self-learning scheme without any ad hoc assumptions or empirical formulations. Starting from an unbiased situation such a scheme will find the optimum with very few iterations.

Slab Thickness = 10 mfp			Slab Thickness = 20 mfp		
Iteration	α	$\Delta\alpha$	Iteration	α	$\Delta\alpha$
0	*0.000*	*+0.573*	0	*+0.000*	*+0.457*
1	*0.573*	*–0.183*	1	*0.457*	*+0.006*
2	*0.390*	*+0.053*			
3	*0.443*	*+0.003*			

Table I. Example of an an iteration approach rendering optimal α-values (biasing factors) for two typical particle deep penetration calculations applying the exponential transform algorithm.

Conclusions: This paper illustrates the application of differential operator sampling in developing a new technique to estimate optimal biasing parameters in non-analog Monte Carlo simulations. Although the test problems involve only the exponential transform as a variance reducing technique, the present scheme can be extended to a wide variety of non-analog simulations including weight dependent games. The overall methodology and application provide a well defined approach to estimate optimal biasing parameters to ensure rapid convergence in self-learning Monte Carlo simulations.

References:

1) H.Rief, J.Comput.Phy., **111**, 33 (1994).
2) H.Rief, Ann.Nucl.Energy, **11**, 455 (1984).
3) H.Rief, "Monte Carlo Uncertainty Analysis" in CRC Handbook on"Uncertainty Analysis", CRC Press, Boca Raton, FL, (1988).
4) H.Rief, Prog.Nucl.Energy, (to be published)
5) R.Y.Rubinstein, "Monte Carlo Optimization, Simulation and Sensitivity of Queuing Networks", John Wiley and Sons., (1986)
6) I.Lux and L.Koblinger, "Monte Carlo Particle Transport Methods: Neutron and Photon Calculations", CRC Press, Boca Raton, FL, (1991).
7) M.Koda, Int.J.Systems Sci., **23**, 2187 (1992).
8) P.K.Sarkar and M.A.Prasad, Nucl.Sci.Eng., **70**, 243 (1979).
9) P.K.Sarkar and M.A.Prasad, Nucl.Sci.Eng., **74**, 52 (1980).
10) I.Lux, Nucl.Sci.Eng., **84**, 388 (1983)

UNCERTAINTY ANALYSIS FOR SOME ACTINIDES AT GROUNDWATER CONDITIONS

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Introduction

Computer calculations are used for many different purposes and important decisions may be influenced by their result. Therefore it is important to know how reliable the results are. The source for the uncertainties in the result may depend on several factors such as pure miscalculations, incomplete understanding of the simulated process and uncertainties in the indata to the program [1]. In the last case the effects may be detected with some numerical uncertainty/sensitivity analysis technique. Several such techniques exist [2, 3], but the work presented here is focused on the application of simple Monte Carlo (MC) sampling. This technique may be favoured for several reasons, e.g. it is easy to use if the number of variables is great and it is easy to perform. Unfortunately it may be difficult to make a sensitivity analysis from the result of a MC sampling of many variables. Therefore the approach adopted makes the analysis in three steps. First a preliminary sensitivity analysis, secondly an uncertainty analysis and thirdly, a stepwise regression based on the result of the uncertainty calculations.

Method

The uncertainty and sensitivity calculations presented in this paper are made with the SENVAR package [4]. The factors included in the analysis are stability- and solubility constants, pH, pe and temperature. The solubility calculations are performed with the thermodynamical equilibrium program PHREEQE [5] and database [6,7]. As aqueous phase a reference water from the Äspö site, was used [8,9].

At least two hundred variables are usually needed for a realistic calculation in a natural water. Therefore a preliminary sensitivity analysis is necessary to start with. The most important factors from that analysis is transferred to the uncertainty analysis where also a stepwise regression is made.

Sensitivity analysis

In the sensitivity analysis one factor is kept constant for a given number of solubility calculations. The variance in the results is the calculated. This value is then divided with the corresponding mean solubility in order to normalise it. These steps are repeated for every factor concerned. The factor that gives the smallest normalised variance is deemed the most important and so on. This ordinary method is modified so that in the beginning of the sensitivity analysis ,a random matrix is made. This matrix has one row for each factor and one column for each sub iteration, i.e. the number of iterations when one factor is fixed. Therefore the factors that are not held fixed, will change their values according to pre-set values. Such an approach will give the unimportant factors similar variances and thus make the selection criterion more simple, e.g. not to include factors, which variance has changed less than 1/1000 of the last accepted one, in the uncertainty analysis.

The ranking obtained with this method is only preliminary and somewhat sensitive to the choice of seed to the randomiser function, since the number of iterations is too small to erase such a dependence. However, the most important species are always present.

Uncertainty analysis

The base for the uncertainty analysis is Monte Carlo sampling of the selected factors within each uniformly distributed interval. The uniformity is selected in order not to impose normality on the results.

The results are evaluated in a common way, i.e. statistical estimators such as mean solubility, variance, confidence interval for the mean and confidence interval for the solubility population are calculated. In addition to that an empirical frequency function is plotted.

The solubilities obtained in the uncertainty calculations are also used for a stepwise regression analysis. From that analysis the final sensitivity analysis is made. Usually there is good agreement between the preliminary and final sensitivity analysis, thus making the credibility of the calculations good.

Results

Table I shows the mean solubility, the confidence interval, the largest and the smallest solubility together with the most important parameters for $Pu(OH)_4(s)$. The empirical distribution frequency for the calculation presented here are shown in Figure I.

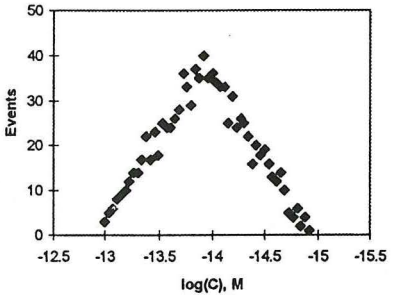

Figure I, The empirical distribution frequency for: $Pu(OH)_{4(s)}$

Table I. Uncertainty result for $Pu(OH)_{4(s)}$. Solubilities in mol/l.

Confidence interval for the mean (95%)	3.08E-08± 4.12E-09
Min;Max solubility	2.03E-09; 3.13E-07
Important parameters	$Pu(OH)_{4(s)}$ $Pu(CO_3)_3^{2-}$ pe Pu^{3+}

The parameters listed in Table I are the ones for which uncertainties in their thermodynamical data will afflict the calculated solubilities the most. The calculated solubilities in Table I fall within the expected range, but expected aqueous species should be $Pu(OH)_4$ (oxidising conditions) and Pu^{3+}, $PuOH^{2+}$, $PuCO_3^+$(reducing conditions) [10]. This shows that the chemically important species not always are those that are the species for those uncertainties in the thermodynamic data are of importance to the calculated result.

The above given results will be further discussed in the full paper together with calculations on U, Np, Th, and Am.

Conclusions

Results in this study shows that the parameters of importance as a result of S/U-analysis will not necessarily coincide with the species of chemical importance.

Uncertainty and sensitivity analysis can be used to give information about parameters of importance in a given system.

This can be used in the Safety analysis for storages of hazardous substances to show which parameters needs to be checked for errors or eliminated their importance.

References

1. Ekberg, C., "Uncertainties in Safety Analysis, A Literature Survey", SKI report 95:17, Swedish Nuclear Power Inspectorate (SKI), Stockholm, 1995.
2. Helton, J. C., "Uncertainty and sensitivity analysis thechniques for use in performance assessment for radioactive waste disposal", Reliability Engineering and System Safety, 42, p. 327-367, 1993.
3. Iman, R. L., Helton, J. C., "Comparison of Uncertainty and Sensitivity Analysis for Computer Models.", Rep. NUREG/CR-3904, Sandia National Laboratories, Albuquerque, NM, 1985.
4. Ekberg, C., "SENVAR: a Code for Handling Chemical Uncertainties in Solubility Calculations", SKI report 95:18, Swedish Nuclear Power Inspectorate (SKI), Stockholm, 1995.
5. D. L. Parkhurst, D. C. Thorstenson, L. N. Plummer, "PHREEQE computer code, version current, August 3, 1984. Changes: a/ NEA DB 17/12/1984, Y Yamagushi, b/ Dept. of Nuclear Chemistry, CTH, 850705, L. Fridemo (adaption to IBM PC+clones, Microsoft FORTRAN 77)
6. K. A. Bond et al, "HATCHES 5.0 - The HARWELL/NIREX Database", Harwell Laboratory, Oxfordshire OX11, ORA, UK, 1992.
7. I. Grenthe, J. Fuger, R.J. Konings, R.J. Lemire, A.B. Muller, C. Nguyen-Trung, H. Wanner, (H. Wanner and I. Forest (ed)), "Chemical Thermodynamics of Uranium", vol. 1., North Holland, Elsevier Science Publishers B.V., ISBN 0 444 89381 4, (1992)
8. Smellie, J., Laaksoharju, M., "The Äspö Hard Rock Laboratory: final evaluation of the hydrochemical pre-investigations in relation to existing geologic and hydraulic conditions", Swedish Nuclear Fuel and Waste Managment co (SKB), TR 92-31 Stockholm, 1992.
9. Nilsson, A-C., "Groundwater chemistry monitoring at Äspö during 1991", Swedish Nuclear Fuel and Waste Managment co (SKB), progress report, 1992.
10. "SKI Project-90", SKI Technical Report 91-23; Swedish Nuclear Power Inspectorate (SKI), Stockholm, 1991.

DETERMINATION OF THE UNCERTAINTIES OF THE INPUT PARAMETERS AND SENSITIVITY ANALYSIS IN THE CATHARE 2 CODE

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1. Introduction

1.1 Purpose of the paper

This paper presents a methodology for determining the uncertainties of input parameters for French safety code Cathare 2. The input parameters considered here are the ones that cannot be measured directly in facilities, that is to say the constitutive relationships (also known as correlations). On account of this feature it is difficult to calculate their uncertainty.

1.2 Presentation of the Cathare 2 code

Cathare 2 (1) is a best-estimate thermal-hydraulics code, which calculates the consequences of a loss-of-coolant-accident in a nuclear power plant. It was developed by EdF (the French utility), Framatome (the French vendor) and CEA-IPSN (the safety authority).

1.3 A part of a global strategy

The issues presented in this paper are a part of a global strategy, the aim of which is the calculation of the uncertainties of the code predictions. For this, a powerful tool is used: the DASM (discrete adjoint sensitivity method), which calculates, at a low CPU-cost, the derivatives of any output parameter with respect to as many input parameters as required (2).

2. Presentation of the methodology

2.1 Some mathematical definitions and notations

• definition of the input parameters

Let CR be a constitutive relationship, which is an analytical expression of the main variables (pressure,enthalpies, void fraction, velocities,etc.). We denote ε the input parameter associated to this correlation and defined by: $CR = \varepsilon \times CR_{nominal}$. So the nominal value of ε is 1. We are looking for the uncertainty of ε instead of that of CR.

• definition of the uncertainties of the parameters

Precisely, the uncertainties relative to a set of correlations are defined with the covariance matrix of the associated parameters. This matrix is denoted as C. It must be positive definite, i.e. with more than 0 eigen values.

2.2 Setting up of the problem

Let us consider a set of correlations, with their associated parameters ε_k, k=1,d. Separate- effect -test facilities, a priori sensitive to these correlations, are used. They are the facilities used for assessing or establishing the correlations. For each of them, the results sensitive to the set of correlations are considered: they are called responses and de-

noted as R_j, j=1,n.

We write for a response R_j, at the first order:

$$y_j = R_{j,\,code} - R_{j,\,exp} = \left(R_{j,\,code} - R_{j,\,true}\right) + \left(R_{j,\,true} - R_{j,\,exp}\right) \qquad (1)$$

that is to say: $y_j = \gamma_j^T (\varepsilon_{j,\,nominal} - \varepsilon_j) + e_j \qquad (2)$

where e_j is related to the experimental uncertainty. Its distribution is assumed to be normal: $e_j \sim N(0,\sigma_j^2)$. σ_j^2 is known.

and $\gamma_j^T = \left(\frac{\partial R_j}{\partial \varepsilon_1}, \ldots, \frac{\partial R_j}{\partial \varepsilon_d}\right)$ is the d-vector given by the DASM.

ε_j is the d-vector of the optimal values of the d parameters when considering the R_j response. It is unknown.

Let us consider the set of n responses R_j, j=1,n. The n $(\varepsilon_{j,1},\ldots,\varepsilon_{j,d})$ vectors are a sample of $\varepsilon=(\varepsilon_1,\ldots,\varepsilon_d)$. We assume that ε has a normal distribution, the parameters of which (mean vector and covariance matrix) are unknown. Particularly, the covariance matrix is the unknown C matrix.

The problem is that the ε_j n-sample is unknown: it is only indirectly given by the y_j n-sample. So the problem is as follows: determine the covariance matrix of $\varepsilon = (\varepsilon_1,\ldots,\varepsilon_d)$, knowing only the y_j n-sample, j=1,n.

2.3 The methodology

It comes from (3). It is an iterative algorithm with two steps at each iteration. Let $C^{(i)}$ be the covariance matrix of ε at the i^{th} iteration. Then the $C^{(i+1)}$ covariance matrix is obtained as follows:

- expectation step (E-step): for one response R_j, it gives the parameters (mean vector and covariance matrix) of the normal distribution of ε_j, after observation of y_j (a posteriori distribution). For this, we use Bayes' theorem on conditional probabilities. We have

$$\varepsilon_j^{(i)} \Big| y_j \sim N\left(C^{(i)}\gamma_j \frac{y_j}{\gamma_j^T C^{(i)} \gamma_j + \sigma_j^2},\; C^{(i)} - \frac{C^{(i)}\gamma_j\gamma_j^T C^{(i)}}{\gamma_j^T C^{(i)} \gamma_j + \sigma_j^2} \right) \qquad (3)$$

the mean vector is denoted as $\hat{\varepsilon}_j^{(i)}$ and the covariance matrix as $C_j^{(i+1)}$.

- maximization step (M-step): it uses the principle of maximum likelihood: an estimation of $C^{(i+1)}$ is $\frac{1}{n}\sum_{j=1}^{n} \varepsilon_j^{(i)} \varepsilon_j^{(i)T}$.

Knowing that the expected value of $\varepsilon_j^{(i)}\varepsilon_j^{(i)T}$ is:

$$E\left(\varepsilon_j^{(i)}\varepsilon_j^{(i)T}\right) = \hat{\varepsilon}_j^{(i)}\hat{\varepsilon}_j^{(i)T} + C_j^{(i+1)} \qquad (4)$$

we obtain the following relationship between $C^{(i+1)}$ and $C^{(i)}$:

$$C^{(i+1)} = C^{(i)} + \frac{1}{n}\sum_{j=1}^{n} \frac{C^{(i)}\gamma_j\gamma_j{}^T C^{(i)}}{\gamma_j{}^T C^{(i)}\gamma_j + \sigma_j{}^2}\left(\frac{y_j{}^2}{\gamma_j{}^T C^{(i)}\gamma_j + \sigma_j{}^2} - 1\right) \qquad (5)$$

Each iteration of the algorithm increases the likelihood of the ε_j sample. The convergence is monotonic and rather rapid. The obtained C matrix is always positive definite.

3. Application to three parameters

3.1 The results

The three considered parameters are

- ε_1: relative to liquid-interface heat exchange (interface between vapour and liquid phases)
- ε_2: relative to friction between vapour and liquid phases
- ε_3: relative to wall-liquid friction

Three analytical experiments are chosen for calculating the covariance matrix of these parameters. One parameter is relevant for each experiment. Its standard deviation is calculated by considering only the corresponding experiment. We find:

$\sigma_{\varepsilon 1} = 1{,}18$, $\sigma_{\varepsilon 2} = 0{,}80$, $\sigma_{\varepsilon 3} = 0{,}17$

When considering the three parameters and the three facilities together, the C matrix is:

$$C = \begin{bmatrix} 1,42 & -0,26 & -0,13 \\ -0,26 & 0,61 & 0,03 \\ -0,13 & 0,03 & 0,01 \end{bmatrix}$$

corresponding to the standard deviations $\sigma_{\varepsilon 1} = 1{,}19$, $\sigma_{\varepsilon 2} = 0{,}78$, $\sigma_{\varepsilon 3} = 0{,}11$ and to the correlation coefficients $\rho_{12} = -0{,}28$, $\rho_{23} = 0{,}37$, $\rho_{31} = -0{,}25$.

3.2 Comments

The results for the standard deviations are close to those obtained by considering only one parameter and one facility. It means that considering experiments where a parameter is not relevant , does not modify its standard deviation. So later, it will be possible to consider together the set of all the correlations of the code with all the corresponding facilities.

Moreover two items were checked for this study:

i) if any one response is suppressed, the results are always very close: the results have converged with respect to the number of responses.

ii) the results are not sensitive to the number of responses per facility, if, nevertheless, this number is high enough.

References:

(1) F. BARRE and al.: New developments in the CATHARE 2 code.NURETH 6, Grenoble, France, October 5-8, 1993.

(2) A. OUNSY, F. de CRECY, B. BRUN: The adjoint sensitivity method; a contribution to the code uncertainty evaluation, Nucl. Engrg. Des. 149 (September 1994) 357-364.

(3) A.P. DEMPSTER, D.B. RUBIN, R.K. TSUTAKAWA: Estimation in Covariance Components Models, Journal of the American Statistical Association, June 1981, Vol 76, Number 374

MayDay. A Code to Perform Uncertainty and Sensitivity Analysis. An application to I^{129} in PSACOIN Level_E exercise.

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ABSTRACT

1.- INTRODUCTION

During the last months a software tool has been developed at the Cátedra de Tecnología Nuclear of the Universidad Politécnica de Madrid (CTN-UPM) to perform Uncertainty and Sensitivity Analysis (UA-SA) on computer models, in the framework of a probabilistic approach to Performance Assessment of Nuclear Waste Repositories. Nevertheless this tool is intended to be useful for any kind of computer model that tackles a problem from a probabilistic point of view. MayDay implements the most common and well-known UA and SA techniques in a user-friendly environment. As a first test case for this tool the study of doses due to I^{129} in the PSACOIN Level_E exercise has been considered. This study has been specially focused on SA.

2.- MayDay AS A SOFTWARE AND STATISTICAL 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 throgh a graphic user interface, X/Windows under Motif, and a carefully designed core that optimizes runtime and CPU resources. MayDay has been developed mainly in C, though there are also some calculation modules in FORTRAN77. 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 important information about the simulations. The data from that file are read as they are needed in the work sesion so that execution speed is highly increased.

MayDay, as a UA tool to study samples, includes general statistics (mean and its possible confidence intervals, variance, geometric mean,...), order statistics with their confidence intervals, it also includes histograms and empirical distribution functions with the Kolmogorov confidence band. Kolmogorov, chi-square and Lilliefors tests are included to check the fit of samples to sampled distributions. The Shapiro-Wilk test is also included to check sample mean convergence to the normal distribution.

Mayday, as an SA tool, includes techniques to study the sensitivity of a single output variable to a single input variable, like the statistics of Pearson and Spearman (related to simple linear regression), and the statistics of Mann-Whitney, Smirnov, Cramer-Von Mises, t, Kruskal-Wallis, and the Smirnov test for k subsamples, among others. MayDay allows also to see the sample of any variable ordered according to the run number or according to the ranks of the observations. It also includes techniques to study the sensitivity of one

single output variable to several input variables like the statistics related to standardized linear regression (PCC,SRC,PRCC and SRRC), the sensitivity measures considered in the Fourier Amplitude Sensitivity Test (FAST), and the estimators developed at the CTN-UPM to measure the change in the means and variances of output variables associated to changes in the distribution of input variables. Scatter plots and contribution to the mean plots are also included. Finally, several tools are implemented for the application of variance reduction techniques: Stratified proportional random sampling, stratified optimal random sampling, LHS, and importance sampling.

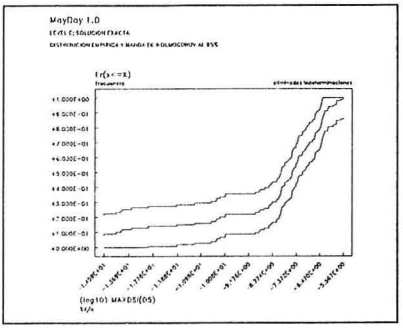
3.- THE STUDY OF I^{129} IN THE PSACOIN LEVEL_E EXERCISE.

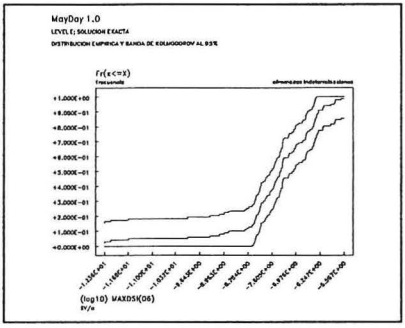
The PSACOIN level_E exercise has been selected to perform a first study with MayDay. This is a widely knowm problem suggested in the PSAC of NEA/OECD. This problem has been simplified so that only one radionuclide, I^{129}, has been considered. It is assumed that a dimensionless repository with an inventory of I^{129} begins to release the contaminant at a constant fractional rate, RELRI (a^{-1}), after a time, CONTIME (a), in which no release happens. The contaminant is transported by groundwater through two consecutive geosphere layers with lengths PATHL1 (m) and PATHL2 (m), and retardation coefficients RETF1I (-) and RETF2I (-), at constant velocities FLOWV1 ($m \cdot a^{-1}$) and FLOWV2 ($m \cdot a^{-1}$). The contaminant leaving the second geosphere layer enters a stream with a given volumetric flow, STFLOW ($m^3 \cdot a^{-1}$), from which the critical group obtains drinking water. The specific equations of this problem, as well as the distributions of the nine uncertain input variables involved, may be found in reference /1/. The output variables studied are the doses at six specific time points (1.E+4, 2.E+4, 5.E+4, 1.E+5, 2.E+5, and 5.E+5 a), DOENTI(0i) - i=1,....,6 - ($Sv \cdot a^{-1}$), the maximum dose up to those time points, MAXDSI(0i) - 1=1,....,6 - ($Sv \cdot a^{-1}$), the maximum dose in the whole simulation period, DOSMAX(01), and the time point in which that maximum happened, TDOSMAX(01).

The problem was solved with the Laplace transform algorithm developed by Robinson and Hodgkinson /2/ and implemented in SYVAC3. A 100 observation random sample was obtained, and doses below 1.E-15 $Sv \cdot a^{-1}$ were set to 0. The first task that was developed was to check the input data that were used in the simulation. Two types of analyses were done: To check if the data fitted the distributions they were sampled from, and to check the independence hypothesis between the seven samples. To perform the first analysis, the Kolmogorov test was applied to each sample. Significative departures from the sampled distributions were found in the case of FLOWV1 and RETF1I, with respective critical levels of 0.014 and 0.02. The probability of this situation is approximately 0.063. To perform the second type of analysis Pearson and Spearman tests were applied to the 36 possible nontrivial couples of input variables. RETF2I and STFLOW showed slightly significative degrees of correlation in the raw values and in the ranks (0.243 and 0.23), moreover, RELRI and STFLOW showed a slightly significative correlation coefficient in the ranks (-0.234). The probabilities of two spureous correlations in the ranks and one in the raw values are about 0.275 and 0.3. As a conclusion of these studies it was concluded that the samples are not the best that could be obtained, but there is not evidence enough to say that they were generated under hypothesis different from those postulated.

Although a large work has been done in the characterization of all the output variables, only the main features will be shown in this abstract. The fractions of null doses were never below 29%, and the non-null part of those doses spread though several orders of magnitude (8 - 9). Another important conclusion of the UA is that, in this case, to work with a sample of 100

observations is to be far from convergence in the study of several output variables. A clear convergence of the series of variables MAXDSI(0i) to DOSMAX(01) as time increases was also detected, as expected. An important result is obtained when studying the relationships among those variables. Very strong correlations in the raw values were found among DOSMAX(01),MAXDSI(06) and MAXDSI(05). The correlation with MAXDSI(02) falls to about 0.5, and MAXDSI(01) is only slightly correlated (0.30) with MAXDSI(02). Nevertheless, when the Mann-Whitney statistic is applied, it is observed that the non-null part of MAXDSI(01) is related to the highest values of MAXDSI(0i) - i=2,...,6 - and DOSMAX(01). In other words, runs that produce non-null doses up to 1.E+4 a produced maximum doses up to posterior time points among the highest, which means that an important fraction of the highest maximum doses happened at early times. The study of the empirical distribution functions of these variables shows also the existence of a clear cut point about 1.E-9 $Sv \cdot a^{-1}$ that divides the populations of these variables in two subpopulations: that in which the maximum dose has happened and that in which that value has not been reached. The latter region spreads through six orders of magnitude, while the former spreads through only three and a half orders of magnitude.





Figures 1 and 2.- *Empirical distribution functions for maximum doses up to 2.E+5 and 5.E+5 a.*

Due to their specific interest, only the results related to standardized linear regression and to FAST will be here reproduced. When regression techniques are applied on the raw values, no good result is obtained, with coefficients of determination below 0.41 in all the cases. Those values are low enough to consider useless any further analysis. Results are quite better when variables are transformed to their ranks (so that monotonic relationships are studied). In the case of the doses at the six time points studied, it may be shown that the process is totally controled by the parameters that characterize the transport through the first geosphere layer, specially FLOWV1. In the case of the maximum doses up to the six time points considered, the process is controled by the same variables; nevertheless, at about 1.E+5 a, STFLOW's importance begins to grow, and at 5.E+5 a it is the most important variable. The reason for that growing importance with time is the increasing fraction of observations in the subpopulation with the highest values. In order to apply the FAST technique, it was necessary to run the simulation code 323 times with the inputs needed by this technique. Only two variables were identified as important by FAST: FLOWV1 and STFLOW. Both in the case of doses at time points and in the case of maximum doses up to those time points, FLOWV1 was more important at early times, while STFLOW was more important at late times.

4.- REFERENCES

/1/ NEA/OECD; "PSACOIN Level_E Intercomparison". Paris. 1989.

/2/ P.C. Robinson and D.P. Hodgkinson. "Exaxct Solutions for Radionuclide Transport in the Presence of Parameter Uncertainty." Radioactive Waste Management and the Nuclear Fuel Cycle. Vol 8, number 4, pp 283-311. 1987.

5.- ACNOWLEDGEMENTS:

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SENSITIVITY, UNCERTAINTY, AND DECISION ANALYSES IN THE PRIORITIZATION OF RESEARCH

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Introduction

The objective of this paper is to describe the role that decision analysis can play in directing the data gathering efforts and design considerations related to complex technical systems. Decision analysis can be used in conjunction with established system models and with other analytic techniques including sensitivity and uncertainty analyses.

Sensitivity analysis refers to techniques that provide measures of the changes in the output of a model that are attributable to changes in the inputs. Often the measures are in relative terms such as percentage change in the output divided by a percentage change in an input or inputs. Such measures may be conditional of the values of other inputs or they may be averaged or integrated over a range of values. Sensitivity methods can be applied to both deterministic and probabilistic models such as those used in probabilistic safety assessment.

Uncertainty analysis provides measures of the uncertainty in output that are attributable to the uncertainty in the inputs. In is applicable to probabilistic models and to deterministic models that are exercised in a probabilistic manner. Measures of uncertainty importance are somewhat more difficult to conceptualize than sensitivity measures. One example of such a measure is the correlation ratio which measures the expected reduction in the variance of the output variable if an input variable's value true value could be determined to be some fixed but unknown value. Such a measure is dependent on both the model and the choice of input distributions.

Decision analysis provides measures of the benefits that can potentially be achieved by making changes to the systems (changes that are reflected in changes in the model) and/or changes to the input distributions to the model. For example, one could change the a nuclear power system by the addition of redundant diesel generator. By applying value measures to the model output both with and without the design modification, a decision can be reached on the worth of the modification. A more complex application is to the value of gathering date that will refine knowledge about the system's safety. Data gathering requires expressions of what is known now, of the potential outcomes of the data gathering activity, and the potential states of knowledge subsequent to the acquisition of the data.

Sensitivity, uncertainty, and decision analyses can be used together to improve the understanding and performance of a system. An application of these techniques has been made to the Waste Isolation Pilot Plant (WIPP), a nuclear waste repository in the Southwest United States. The goal of this application is to provide a prioritization for expenditures on research activities and design modifications. The decision maker (US Department of Energy) is provided with measures of cost, time, and the likelihood of successful licensing for various portfolios of research activities and design

modifications.

Risk Analysis and Performance Assessment

Central to this discussion is a model of the system under study. Sensitivity and uncertainty analyses assume the existence of such of a model. This is not true in decision analysis where the process often generates a "requisite" model that may contain much less detail than the corresponding systems model. It will be assumed that a computer implemented system model exists, however, and that the decision analysis exercises this model in a coordinated manner to address particular decisions.

The systems model is exercised by selecting inputs. For both uncertainty and decision analyses, these inputs are selected according to probability distributions that reflect the uncertainty in the input. Most often, this uncertainty is attributable to a lack of knowledge about a parameter that could, at least conceptually be known with certainty. It may also be, however, that natural variation makes the parameter essentially unknowable. In contrast, sensitivity analysis can be performed without reference to any probability distributions or it can be performed on the parameters of such distributions.

When a model is a exercised in a probabilistic fashion, the output is a random vector or perhaps a set of random functions. One representation of model output involves the separation of uncertainties attributable to knowledge uncertainties from uncertainty that is natural or nonreducible. This type of representation has played an important role in a number of US risk assessments including that for the WIPP.

Exercising the model produces a sample of values from the uncertainty distribution of the model output. There are various ways in which this output can be compared to criteria. For example, the criteria may be stated in terms of a mean value. Conversely, the criteria may be in probabilistic form. The US criteria for transuranic waste disposal calls for no more than a one in ten chance of exceeding one standardized unit of release to the environment. This criteria requires, then, that the model output is in the form of a CDF or that a CDF can be created from the output.

Decision analysis

While the end result of decision analysis is the recommendation of an optimal strategy, the recommendation itself is subject to sensitivity analysis. This is, of course, only proper since any model based analysis provides only an approximation to the decision to be addressed. It will be kept in mind, then, that decision analysis does not "make" decisions, its intent is provide information in a form useful to the decision maker.

Decision analysis for complex systems can be performed by using the decision analysis paradigm to exercise the systems model rather than manufacturing a decision structure from the ground up. There are several advantages to such an approach. First, the systems models are often well understood by the parties involved in the decision and therefore trusted. Second, the level of effort required to build an adequate representation of the system exclusively for the decision analysis can be substantial. Such effort is avoided by adopting the systems model. On the down-side,

the systems model may be computationally intensive and, because a decision analysis will require a large number of evaluations, the computational time and cost may be excessive.

One common form of a decision tree is the two-stage tree with the first stage being a decision to implement a certain set of information gathering activities and the second stage being a terminal decision based upon the outcome of the first stage. Two distinct types of uncertainties are represented in this tree structure. One type of uncertainty is about the outcomes of the information gathering activities. The other type of uncertainty relates to the knowledge that one would have given a particular outcome of the information gathering activity.

A complete decision analysis requires a utility function to measure the goodness of various outcomes. The utility function may have a vector domain with the elements being such things as health effects, environmental damage, costs, time, etc. If the analysis is being done to demonstrate compliance, then an indicator may be of compliance may then be used as a measure of utility. The expected value of the indicator then provides a measure of the value of an information gathering strategy.

There are several key components to decision analysis. Central to understanding and emulating the system is the risk assessment model. The choice of input distributions is also key. Here the distributions must be expressive of the uncertainties in the outcomes of the information gathering activities and expressive of the residual uncertainties conditional on the various potential outcomes of the activity.

The decision analysis produces measures of value for each strategy. In a risk assessment that is directed at demonstrating compliance, this measure can be the probability of demonstrating compliance. This probability can then be compared to cost and time measures to determine an optimal portfolio of activities to undertake.

The WIPP Systems Prioritization Methodology

Recently, an application of decision analysis was made to the WIPP as a decision-making aide in selecting activities to be conducted prior to a submission of an application for licensing. The study was conducted in two stages, SPM-1 and SPM-2 (Systems Prioritization Methodology 1 and 2.)

One of the more unusual features of the SPM methodology is the use of baseline distributions rather than more traditional prior distributions. The baseline distribution is roughly defined as the least conservative distribution that could be successfully defended in a court of law given the present state of scientific knowledge. For various reasons, this choice became troublesome and required refinement and redefinition as the project proceeded.

One the most difficult activities in implementing SPM was the acquisition of distributions for experimental outcomes. Scientists and engineers do not seem accustomed to thinking about the various potential outcomes of their studies. Rather, they are comfortable in thinking about outcomes as successes and failures -- the experiment succeeds and confirms the scientist's beliefs or it fails and does not

produce defensible results. Some difficulties were also encountered in obtaining conditional distributions for parameters.

One constraining factor ins both SPM-1 and SPM-2 was the amount of computer time that was required to evaluate the many combinations of activities and the potential outcomes of these activities. So that the calculations could be done within cost and time budgets, a fairly coarse level of refinement was used with respect to the outcomes of activities. Moreover, a computational strategy was developed that avoided making large numbers of evaluations with portions of the performance assessment model that are most expensive to run.

SENSITIVITY ANALYSIS IN DECISION ANALYSIS

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Many activities in quantitative modelling lead to comparisons of a set A of actions, designs or alternatives a according to an evaluation function $\Psi(a, w)$, which depends on parameters w. We might be interested in checking the sensitivity of the output of our analysis to changes in the parameters.

We have been developing a framework to deal with such problems (1). The framework was developed mainly for decision analytic contexts. Our aim here is to describe it, with emphasis on recent developments. We shall also describe an application to a radiation protection problem and explore extensions to more general settings.

1 The basic framework

We start with the typical decision analytic framework. Assume that A is a finite set of alternatives. The evaluation function is the expected utility which depends on parameters related to the probability distribution and to the utility function. We assume that there is some imprecision about these parameters, modelled by constraints $w \in S$. There is also some initial guess w_0, and the alternative maximising $\Psi(., w_0)$ is the candidate optimal alternative. We want to check, however, the impact of w on that optimal alternative.

2 Filtering phase

We consider first a set of filters which help us to detect the alternatives that are worthwhile retaining in the analysis.

Nondominated alternatives These are alternatives such that there is no other alternative which is better for all possible parameters $w \in S$.

Potentially optimal alternatives These are alternatives that are optimal for some $w \in S$.

Adjacent potentially optimal These are alternatives that share optimality with the current optimal alternative for some $w \in S$.

All these alternatives may be discovered via mathematical programming (2). At the end of this phase we end up with a set of alternatives on which the decision maker should focus attention. As a byproduct, we also obtain estimates of potential losses of optimality. If these are not considered too important, we might declare that the problem is solved.

3 Sensitivity Analysis phase

The purpose of this phase is to detect changes in the parameters leading to changes in the optimal alternative. We use two types of tools.

Distance analysis We use distances to detect parameters closest to w_0 leading to the current optimal alternative being outranked by some other alternative. Again we use mathematical programming to solve this problem (2).

Differential analysis To speed up computations, we do a similar approach based on linear approximations to the evaluation functions. In more complex settings, we have to appeal to Fréchet derivatives.

4 Display of results

The information obtained above is very rich and has to be displayed conveniently to convey all its meaning to the decision maker. Graphs, sensitivity measures and interpretations are provided (1).

5 Implementation

The framework is embedded naturally in a cycle of modelling, optimisation, sensitivity analysis until the model is requisite.

The solution of a large number of mathematical programmes is potentially required. Some of these are nonconvex and global optimisation is necessary to provide reliable sensitivity information. Consequently, the computational load may be heavy. We have undertaken a number of implementations of the framework in order to assess its computational viability via changes to the high-level sensitivity analysis algorithm, to the detailed algorithms used to solve various subproblems and to the formulation of those subproblems (3). We also have investigated a coarse-grain parallel approach, using the processor farm model, in which complete mathematical programming problems are solved on a single processor (4).

We have concentrated on cases in which $\Psi(a, w)$ is either linear or bilinear and in which S is defined by linear constraints. For such cases general purpose packages have been constructed which allow distance analyses to be performed in L_1, L_2 and L_∞ metrics. For more general cases, problem-specific software needs to be written. Our results suggest that a PC-based sequential implementation is viable for realistic sized linear and bilinear discrete MCDA models.

6 A case study in radiation protection

As an illustration of our framework, we discuss its application to a hypothetical radiation accident. This scenario was explored at a decision conference undertaken on behalf of the Nordic Cooperation Organisation (5). A number of strategies for medium and long term protective actions were investigated in terms of six criteria using a multi-attribute value model.

7 Extensions

We shall describe two possible extensions.

7.1 The continuous case

In many cases, the set of alternatives is continuous. Many of the ideas above can be extended. For example, the set of nondominated alternatives can be approximated through simulation. First, draw a sample of alternatives and apply the methods above. Use the resulting set as an approximation to the nondominated set, perhaps with the aid of some smoother. This smoother can be used to define stopping rules to decide when to stop sampling.

7.2 The implicit function case

In the above, it was implicitly assumed that we had an explicit expression for the evaluation function. We have dealt with cases in which this does not hold; for example, influence diagrams.

The case in which the evaluation is obtained with a simulation is also of interest. If this evaluation is cheap, we may apply the previous framework with optimisation methods not using derivatives. When the evaluation is expensive, we may obtain a sample $\{\Psi(a_i, w_i)\}_{i=1}^n$, fit a regression metamodel and appeal to the previous framework.

8 References

(1) Rios Insua D, Sensitivity Analysis in Multi-objective Decision Making. Lecture Notes in Economics and Mathematical Systems No.347, Springer Verlag (1990)
(2) Proll LG, Rios Insua D and Salhi A, Mathematical programming and the sensitivity of multi-criteria decisions, Annals of Operations Research, 43, pp.109-122 (1993)
(3) Proll LG, Rios Insua D and Salhi A, An improved implementation of an algorithm for sensitivity analysis in MCDA (in preparation)
(4) Proll LG, Rios Insua D and Salhi A, A parallel implementation of a mathematical programming framework for sensitivity analysis in MCDM, presented at APMOD93 Applied Mathematical Programming and Modelling, Budapest, January 1993 (1993)
(5) French S, Walmod-Larsen, O and Sinkko, K Decision conferencing on countermeasures after a large nuclear accident, Report Riso-R-767(EN), Riso National Laboratory, Roskilde, Denmark (1993)

Economic risk versus technological risk in large investment projects

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Abstract

The financial feasibility of large investment projects (such as investments in gas transmission and power systems) has many aspects. Usually, this multi-facetted problem can not be modeled as a single optimization problem; instead the multiple aspects are modeled separately: demand, supply, prices, investment cost submodels. Each aspect may require a large, nonlinear submodel. The results per submodel used in the final evaluation are often limited to one or a few variables, which combine all the submodel information; for example, the result of the demand model is the sum of the demand per customer type, each type being modeled separately. The feasibility of the investment project is then judged by combining the results of the various submodels for the 'base case' values of all model inputs.

The preferred criterion for project evaluation is the expected Net Present Value $E(NPV)$. However, for the decision makers this certainty information is not sufficient; they also like to know the financial risk they are taking.

The project's risk is sometimes defined as the variance of the NPV, $V(NPV)$. A method to assess this risk on the project level is known as risk analysis or risk simulation, which estimates the $f(NPV)$, the probability distribution of the NPV. That distribution is obtained by introducing distributions for the model inputs or intermediate variables. Many software packages (such as @RISK for Lotus 1-2-3 and Crystal Ball) facilitate this type of risk analysis.

Risk analysis may comprise two steps. First, one factor at a time sensitivity analysis is performed to determine which factors are important. Second, for these important variables a probability distribution is assumed, which has to account for the stochastic nature of the problem. In most cases only the marginal distributions of the inputs are assumed, which implies that the input variables are supposed to be independent.

Although this type of risk analysis is appealing, it has theoretical and practical flaws, which may lead to wrong conclusions. Risk analysis also provides insufficient information for the decision maker.

The type of risk analysis described above, is analogous to analyzing the technical or operational risk of an investment. However, technical risk and financial risk are different concepts and require different analyses. For example, consider a gas

transmission system. In its simplest form the technical safety requirement can be formulated as: the chance of a blow up has to be smaller than α, $P(PIPELINE\ BLOW\ UP) \leq \alpha$, with $0 < \alpha < 1$. This requirement leads to technical requirements for various parts of the system, such as, pipeline sections, compressor stations, and city gate stations. These requirements are translated into safety requirements in the form of construction regulations, such as, ANSI/ASME B31.8. If these safety standards are met, the technical risk can be insured (financial risk cannot be insured).

Financial risk analysis starts with the same requirement as technical risk assessment, that is $P(\hat{NPV} \leq 0) \leq \alpha$. However, there is an important difference. The NPV is influenced by other markets, whereas the technical risk is not; a technically safe system remains safe, *independent of other systems*.

Furthermore, the fact that the requirement $P(\hat{NPV} \leq 0) \leq \alpha$ holds, does not say much about the project's risk. Uncertainty about the outcome of a project is not the same as riskiness. Uncertainty and risk only coincide if there is a single project. In case there is more than one project, a project constitutes a risk only in so far as it affects the variability of the total portfolio. This can be illustrated by a well known example, namely insuring a house against fire. The $E(NPV)$ of the insurance is negative; otherwise the insurance company would go broke. The portfolio consisting of the house plus the insurance, has the sure value of the value of the house minus the insurance premium. So the insurance is a good investment, despite its negative $E(NPV)$.

Large investment projects are one shot opportunities, which have an impact on the total economy. This clearly distinguishes these projects from routine investment projects, such as stock market portfolio management or small additional investments for replacement. The information required for the large projects is larger and more ad hoc, and the evaluation period is much longer. For example, a large pipeline system requires analyses of energy market and energy pricing policy for at least the next twenty years. Formulating even a limited number of scenarios is already complicated. It is difficult to obtain probability estimates for the inputs, because of the nature of the problem, which requires estimates of the contemporal and intertemporal correlations.

To obtain such probability estimates one could start rather arbitrary with a triangle distribution. The base case value is then the modus of the distribution, Moreover, a minimum and maximum value for each input has to be established. However, if one bases risk analysis on arbitrary or "estimated" probability distributions, a third step should be added, namely sensitivity analysis of the NPV to the uncertainty in the input distributions. This leads to statements about the reliability of $P(\hat{NPV} \leq 0) \leq \alpha$ of the form "the chance that $P(\hat{NPV} \leq 0) \leq \alpha$ holds is 90%". This concept will be even harder to sell to the decision makers. One could argue that the interpretation of such an elaborate result could be left to the trained analyst. However, this would take away the decision makers control over the decision.

If we assume that all these theoretical and practical problems can be overcome, there is one more issue to be resolved: what is the informational value for the decision maker of knowing that $P(\hat{NPV} \leq 0) \leq \alpha$? This value is limited, because there is no information on what can cause the project to go wrong. Note that if the decision makers can agree upon a suitable value for α for large investment projects, their contribution is no longer required. The decision can be "programmed", and again the decision maker is no longer required.

For large projects an alternative approach can be formulated, which requires no assumptions about (joint) probability distributions of the input variables, and meets the

decision makers information needs better than risk analysis does. This approach is based on the *statistical theory on design of experiments* (DOE). Instead of one factor at a time (as in step one of risk analysis) a more elaborated design (such as factorial designs) is used to analyze the effect of factor changes. These designs allow the analysts to estimate which factors important main effects (first order effects), and which -if any- interactions between factors are important. (Accounting for interactions was one of the reasons for proposing risk analysis.)

We will illustrate this approach by the investment analysis of a large (2 billion U.S. dollars) investment in gas transmission in Indonesia.

Keywords: Sensitivity analysis, Risk analysis, Experimental design, Investment evaluation.

UNCERTAINTY ANALYSIS IN BUILDING THERMAL MODELLING

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Abstract
Two parameter screening techniques, a sequential bifurcation method and a factorial sampling method, have been applied to a building thermal simulation model. The objective of the study was to determine the parameters that contribute the most to the uncertainty in a specific simulation result, that is thermal comfort performance. The results of the two methods are supplementary. Twelve parametrizations of complex physical processes were identified as 'important'. They will receive further consideration in future research.

Introduction
In the final design stages of a building a prediction of the future thermal comfort performance is required. Thermal comfort performance is an index that rates the quality of a building with respect to indoor climate. Thermal comfort depends mainly on the temperature field in the building.
The basis of thermal building simulation consists of solving the temperature field from the heat balance of the building. Spatial discretisation of the temperature field results in an expression for the temperature vector y:

$$\dot{y} = \mathbf{A}y + \mathbf{B}v + f \qquad (1)$$

wherein v denotes the control vector and f is the forcing vector, representing the inputs from outside the system. The matrices A and B comprise the building model parameters. In present day practice building simulation calculations are carried out deterministically.
However, the values of these parameters and inputs will often be uncertain. The sources of this uncertainty can be classified into four different categories:

1. Lack of knowledge about the building details in different stages of the design process.
2. Uncertainty due to spread in manufacture and assembly quality of the building components.
3. Unpredictable behaviour of the future users of the building.
4. Lack of knowledge about some of the underlying physical processes, i.e. parametrizations of processes, that are considered to be too complex to model in detail.

Case study
The comfort performance simulation of a single room in a standard Dutch office building has been used as a case for this investigation. Thermal building simulation has been performed with a dedicated configuration of the finite element toolbox BFEP (1) that has a substantial user base in Dutch design practice. The comfort performance has been calculated according to the guidelines of the Dutch Government Building Agency (GBA) (2,3). In this case only uncertainties in the 82 building model parameters were considered. Estimates of the uncertainty in the model parameters were mainly extracted from literature (4,5). The remaining uncertainty intervals had to be estimated.

A single deterministic simulation of the comfort performance with mean parameter values results in a comfort performance of 105 hours. As the GBA allows a maximum value of 100 hours, this design alternative would probably be rejected in practice. Considering a standard deviation of the simulation result of approximately 40 hours, this seems a contestable decision.

To be able to make better decisions a designer should firstly minimize the uncertainty in his simulation results. Secondly, he should be able to assess the remaining uncertainty.

This paper is dedicated to the first step in minimizing the uncertainties. Several physical processes in the building have been roughly modelled by single (time and state invariant) parameters for reason of simplicity. These simplifications imply uncertainties in the values of these parameters. If these uncertainties make an important contribution to the uncertainty in the comfort performance prediction, modelling refinement and improvement could lead to a reduction of this uncertainty.
To investigate the relative importance of these parameters, a parameter screening has been performed.

Parameter screening
The screening method had to meet a few basic requirements. The screening should yield a qualitative ranking of the parameter importance, the implementation should be simple in this stage of the project and no superfluous information should be produced. On the basis of these requirements two screening methods were selected: sequential bifurcation according to Bettonvil (6) and a factorial sampling method developed by Morris (7).

Sequential Bifurcation assumes that the model can be approximated by a meta model with main effects and first order interactions only. In the screening procedure, all parameters can only accept two values, 'off' and 'on'. Each parameter should be coded so, that if it is switched from 'off' to 'on', the model output does not decrease. At the start of the screening two output observations are made, one with all parameters 'off' and one with all 'on'. Two combinations of the observations are formed that only depend on the main effects. The difference between the corresponding combinations is a (multiple of) the sum of all parameter main effects. This sum is sequentially bifurcated in smaller sums until individual main effects are assessed. The results of the screening with sequential bifurcation are shown in table 1. These results were reached after 25 pairs of simulations.

parameter index	individual effect (bifurcation)	parameters found by factorial sampling	description
16	105	x	ext. convective heat transfer coeff. roof
1	88	x	ventilation rate with outdoor air
8	69	x	int. convective heat transfer coeff. floor
11	51	x	transmission coeff. solar shading
13	46	x	ext. convective heat transfer coeff. window
4	35	x	int. convective heat transfer coeff. facade
2	33	x	indoor relative humidity
9	29		int. convective heat transfer coeff. ceiling
3	27	x	indoor air velocity
14	25	x	ext. convective heat transfer coeff. parapet
5	20	x	int. convective heat transfer coeff. wall
10	17		fraction of solar load to indoor air node
12	15		transmission coeff. window
6	11	x	int. conv. heat transfer coeff. rear wall
22	11		total volume heat capacity
23	10	x	albedo (reflectivity building environment)
33	-	x	heat resistance window air gap
38	-	x	conductivity isolation layer in parapet

Table 1. Results of the two screening methods.

As the validity of the meta model could not be confirmed beyond dispute, a second screening method was applied, that has no reliance on the adequacy of a lower order polynomial meta model: a factorial sampling method. The factorial sampling plans were composed of individually

randomized one-factor-at-a-time designs and the analysis of the results is based on the resulting random sample of observed elementary effects, the changes in the output solely due to changes in a particular input.
An estimate for the mean and standard deviation of the elementary effect for each parameter was calculated from simulation results of four independent random designs. Parameters with either a significant mean or a significant standard deviation were considered important. This method only yields a global ranking of importance. The important parameters are therefore shown in table 1 without rank information. These results required 328 simulations.

Discussion and summary
The two methods show slightly different results. Parameters 33 and 38 were not found by sequential bifurcation. This can be explained from the fact that the simulation output is not monotonous with these parameters. Four parameters, declared important by sequential bifurcation, were not found by factorial sampling. This is probably due to the limited number of independent factorial designs that were subjected to calculation. The results of the two methods can be regarded as supplementary. Twelve of the eighteen important parameters are indeed rough parametrizations of complex physical processes. They will be considered in more detail in future research.

Future research
The first concern in future research will be to examine the sensitivity of these results for the specific building design that is considered. A substitution of several important model parameters by a more accurate representation of the underlying physical process will also be subject of investigation to reduce the uncertainty in comfort performance predictions. A subsequent study will be dedicated to a thorough assessment and modelling of the remaining relevant parameter uncertainties. Finally, a method should be developed to assess the uncertainty in the comfort performance with a minimum of computation time, which could be applied in a design tool for application in practice.

References
1. Augenbroe, G.L.M.; Research-oriented tools for temperature calculations in buildings., Proc. 2nd Int. Conf. on System Simulation in Buildings, Liege. (December 1986)
2. ISO 7730, Moderate thermal environments. Determination of the PMV and the PPD indices and specification of the conditions for thermal comfort. (1994)
3. Brouwers, G.F.M., Linden, A.C. van der; Evaluation of the thermal indoor climate (in Dutch), Klimaatbeheersing 18 v7 p257-264 (1989)
4. Lomas, K.J., Eppel, H.; Sensitivity analysis techniques for building thermal simulation programs., Energy and Buildings 19 p21-44 (1992)
5. Pinney, A.A. e.a.; The choice of uncertainty limits on program input parameters within the applicability study 1 project., Report E/5A/CON/1213/1784, School of the Built Environment, Leicester Polytechnic (1991)
6. Bettonvil, B.W.M.; Detection of important factors by sequential bifurcation., Tilburg University Press, Tilburg (1990)
7. Morris, M.D.; Factorial sampling plans for preliminary computational experiments., Technometrics 33 v2 p161-174 (1991)
8. Janssen, P.H.M., Slob, W., Rotmans, J.; Sensitivity analysis and uncertainty analysis; an inventory of ideas, methods and techniques (in Dutch), Report 958805001, Rijksinstituut voor Volksgezondheid en Milieuhygiëne (1990)

DETECTING THE RELIABILITY OF INFLUENTIAL VARIABLES IN THE SIMULATION BEHAVIOUR OF LARGE NONLINEAR ECONOMETRIC MODELS

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1. Introduction

Computing power has increased enormously over the past 30 years and since computing costs have ceased to be a serious barrier, macromodels have grown from small-scale academic exercises to complex nonlinear models with more than 1000 equations.

The seminal work "Structural Sensitivity in Econometric Models" by Kuh, Neese and Hollinger KNH (1985) suggests strategies and procedures for understanding models and identifying what really counts in determining their behaviour.

In presence of nonlinear models, the approach suggested by KNH requires the analysis of the linearized counterpart of the model. A mild degree of nonlinearity is, of course, a crucial prerequisite for validating the information derived from linearized models so that, practically, analysis of linear models (LIMO) is not always a viable procedure. As shown in Bianchi, Bruno and Cividini BBC (1992), this is the case for some models developed at the Research Department of the Bank of Italy.

In this paper the behaviour of large nonlinear models is considered, and, as an alternative to LIMO analysis, the influential variables are detected through simulation of the nonlinear model. Furthermore, the effects of the predetermined variables, measured in multipliers in elasticity form, are also evaluated with respect to their statistical reliability, thus allowing the model user not only to detect the more influential variables but also to appreciate the statistical reliability of the variables most important in determining the models behaviour.

The proposed analyses involve a large number of independent solutions, so that, as discussed in BBC (1992), numerical intensive computational techniques (NIC) can usefully be applied.

A short description of the computational procedures that have been implemented at the Research Department of the Bank of Italy is included, and the procedures will be strengthened by numerical illustrations on operational models currently used in the Bank.

2. Detecting the Influential Variables

Multipliers, i.e. the changes in the endogenous (dependent) variables in rensponse to those in predetermined exogenous variables, are frequently computed either when validating the model or when using it for policy experiments. In the case of linear models, multipliers can be easily computed by means of analytical formulae. In nonlinear models,

multipliers are computed by means of numerical simulation of the model as the ratio of the changes in the endogenous variable with respect to changes in predetermined variables. At time period (t), the computation of the multiplier of the endogenous variable (i) with respect to the predetermined variable (j) involves two solutions of the model: the so-called control solution and the disturbed solution, i.e. the solution when an increment is given to level of the predetermined variable (j).

Multipliers are frequently transformed into elasticities (in KNH called multipliers in elasticities form). The elasticity is nothing more than the ratio of the relative change in the endogenous variable (i) with respect to the relative change in the predetermined variable (j).

It can be easily shown that, for each endogenous variable, in the simulation period (t), the elasticities with respect to all the predetermined variables of the model sum up to 1.

Using this nice property (share interpretation of the elasticities), it becomes clear how to detect the influential variables: the most influential variables are those with the highest absolute value in terms of elasticity.

3. Detecting the Reliability of the Influential Variables

The reliability of the effects of the predetermined variables can be detected estimating the asymptotic variances of the elasticities. These variances are analyzed in terms of large sample theory by applying the convergence theorem for function of random variables.

If consistent estimates of the structural coefficients (with their covariance matrix) are available, assuming the asymptotic normality of the coefficient estimates, the application of the so-called δ-method (Rao 1973, p. 338) allows an estimation of the asymptotic standard errors (i.e. reliability) of the elasticities.

The computation of the elasticities involves nonlinear transformations of the structural coefficients, but the asymptotic normality can be mantained even with nonlinear transformations provided that they belong to a class of continuously differentiable functions, conditions which are usually satisfied to a large extent in the class of econometric models we are using.

At period (t), given the elasticity (e_{ijt}) of the endogenous (i) with respect to the predetermined (j), applying the δ-method, it turns out:

$$\sqrt{T}\cdot(\hat{e}_{ij}-e_{ij}) \xrightarrow{D} N(0, J\,\Psi J')$$

where

$J=\dfrac{\partial e_{ij}}{\partial \boldsymbol{a}}$ is the vector of the derivatives of (e_{ij}) with respect to all the structural coefficients $(\boldsymbol{a})$ of the model, and Ψ is a consistent estimate of the covariance matrix of the structural coefficients $(\boldsymbol{a})$ of the model.

The derivatives are computed by means of numerical simulation of the model as ratios of finite increments.

REFERENCES

Bianchi, C., G. Bruno and A. Cividini (1992), "Analysis of Large Scale Econometric Models Using Supercomputer Techniques", Computer Science in Economics and Management, Vol.5 pp. 271-281.

Kuh, E., J.W. Neese and P. Hollinger (1985), Structural Sensitivity in Econometric Models, John Wiley & Sons, New York.

Rao, C.R., (1973), Linear Statistical Inference and its Applications, John Wiley & Sons, New York.

MODELLING THE TECHNICAL AND ECONOMIC CONSEQUENCES OF CONTROL STRATEGIES FOR FOOT-AND-MOUTH DISEASE OUTBREAKS IN THE EUROPEAN UNION

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Introduction

Outbreaks of foot-and-mouth disease (FMD) may result in considerable economic losses, especially for countries such as the Netherlands whose livestock industry depends heavily on export of livestock and livestock products. Decisions regarding the control of this type of disease outbreaks comprise a large amount of uncertainty regarding the possible extent of the outbreak (size of the area and number of farms involved) as well as the possibility of export bans set by other countries (which countries, over what period of time, production banned from the entire country or from a region only).

A stochastic simulation model is being developed which calculates the technical and economic consequences of different control strategies for FMD outbreaks taking into account these uncertainties. The model can be divided into three parts: simulation of (a) disease spread between farms, (b) direct costs of eradication and (c) indirect costs due to export bans. In that, simulation of disease spread serves as starting point for the economic calculations. Input parameters on disease spread are especially difficult to obtain, since (data about) epidemics of FMD are scarce. This paper focuses on the use of sensitivity analysis to validate the simulation model for disease spread; which input parameters and distributions have a large impact on the extent of the outbreak. For practical decision making it is then important to get more precise estimates for the most decisive parameters and distributions.

Outline simulation of disease spread

FMD is an extremely infectious virus disease which can affect any cloven-hoofed animal and which spreads through different mechanisms (animals, people, vehicles, air). As set by European Union (EU) law, preventive vaccination is not allowed. In case of introduction of FMD, rapid spread may occur. FMD should be eradicated by slaughtering and destroying affected herds and by installing additional controls, such as radial zones in which movements of animals, people and vehicles are restricted and tracing farms that had contact with infected farms.

In the simulation model Interspread (1), disease spread between farms is modelled via a number of spread mechanisms that operate geographically and that can be subject to a range of control strategies that operate partly spatially as well (e.g. movement restrictions and emergency vaccination). Starting point is the infection of a single farm. From day to day further disease spread is simulated, until no new outbreaks occur. Common random numbers have been applied to reduce variance.

Results simulation of disease spread

A prototype version of the model was used to carry out a first sensitivity analysis. Calculations were carried out for an area of 50*50 km, with the average Dutch farm

density (2 per km^2) and a combination of dairy, pig and mixed farms. The first infected farm was located in the centre of the area. The control strategy applied represents the basic Dutch strategy. Disease spread parameters were based on the values defined for New Zealand (1), except for those that are directly related to the structure/organisation of animal production (e.g. number of movements).

Table 1. Results regarding number of outbreaks for basic scenario and some alternatives.

Scenario	Mean	S.D.	Median	Probability 1 outbreak only	95% percentile
Basic	11.6	9.0	9.0	0.06	32.4
Movements +25%	13.7	10.9	10.0	0.08	38.0
Movements -25%	8.5	7.4	6.0	0.12	23.4
No movements	5.1	3.8	4.0	0.20	14.0
Local spread +25%	13.6	10.6	9.0	0.04	32.9
No local spread	4.8	4.2	3.5	0.22	14.5
Prob of infection +25%	22.4	17.5	20.0	0.04	61.8
Number of farms +100%	11.9	11.9	9.5	0.12	33.6

Table 1 gives some results of the sensitivity analysis (50 replications per scenario). Since the results are rather skewed, next to the mean number of outbreaks, parameters reflecting the spread in outbreaks are presented as well. In the basic situation, on average 1.9 movements are simulated off infected farms per day. A reduction or increase in the number of movements of 25% results in an increase or decrease of the mean number of outbreaks at a similar rate. In case no movements would occur between farms, the extent of the outbreaks is halved. The same effect occurs in case probabilities of local spread were set to zero. When generating movements, a probability of infection is assigned to each movement of 0.5, 0.05 and 0.005 respectively for high (0.17 movements per day), medium (0.59) and low risk (1.14) movements. These probabilities of infection have been chosen arbitrary. Increasing the probability of infection due to movements with 50% has a very large effect on the extent of the outbreak.

Once validated, the model can be used to compare the consequences of different control strategies. This is illustrated here by presenting results for two control strategies. In the basic strategy a so-called restricted area (RA) is installed in which movements are controlled. An RA is a large area that covers all infected farms and a certain area around each infected farm. In the alternative strategy, this RA is not in place, but only single radial zones around each infected farm (as in the basic strategy). Figure 1 shows the cumulative frequency distribution of the number of outbreaks for both strategies (50 replications). Results are shown for two situations: basic and increased number of movements per day off infected farms. For the basic number of movements, in about 40% of the cases both strategies result in only a small number of outbreaks. In those cases, the strategy without RA will be cheaper, since there are less costs involved for farms that have been put on movement control. When the number of outbreaks runs more out of hand, the situation becomes even more worse in case no RA is installed. The reduction in costs of not having an RA will be overtaken by the increase in costs due to much more outbreaks, especially in the situation where the number of movements is increased.

Discussion and conclusions

The results of the sensitivity analysis show that more effort is needed to obtain better information on the probability of local spread and the probability of infection due to

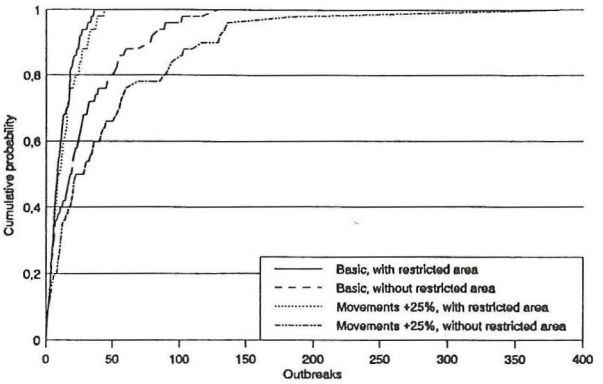

Figure 1. Cumulative probability distribution of the number of outbreaks for scenarios that differ in number of movements and whether a restricted area is put in place or not.

movements of animals, people and vehicles. The probability of an individual farm becoming infected due to local spread off an infected farm is rather low (max. 0.05 per day) but has a large impact on the extent of the outbreak. These parameters, however, were estimated using data of a single epidemic only. The probability of infection due to movements will have to be more related to type of farm and number of animals involved.

To obtain the economic consequences of different control strategies, the results of the simulation of disease spread will be combined with a modified version of the model of Berentsen et al. (2) to obtain direct costs of eradication and indirect costs due to export bans. In analyzing the results of control strategies, decision rules (stochastic efficiency criteria) will be applied to show the impact of various risk attitudes of decision makers in determining what control strategy to apply. The model can be used to test control strategies prior to implementation during an actual FMD outbreak, but can also be used as a research and training tool in periods without outbreaks. In research the influence of farm/animal density, control strategy and disease spread parameters on the extent and costs of outbreaks can be examined.

Acknowledgements

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References

(1) Sanson, R.L., 1993. The development of a decision support system for an animal disease emergency. PhD-thesis. Massey University, Palmerston North, New Zealand. 264 pp.

(2) Berentsen, P.B.M., Dijkhuizen, A.A. and Oskam, A.J., 1990 Foot-and-mouth disease and export: An economic evaluation of preventive and control strategies for the Netherlands. Wageningen Economic Studies No. 20, Wageningen Agricultural University, 89 pp.

THE SENSITIVITY OF FORCE ESTIMATION IN FLEXIBLY SUPPORTED MACHINES

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The analysis of the vibrational behaviour of turbo machinery is a topic of great importance in most process industries and particularly in power generation. Apart from the need to design machinery to operate within acceptable limits, dynamic models are now used to great effect in the diagnosis of operational difficulties. In principle it should be possible to develop a suitable model from finite element techniques, but there are a number of practical difficulties. It is often found that similar units, built to the same drawings, display substantially different vibrational behaviour. The most attractive option to elucidate the foundation's dynamic properties, is to extract information from the response of the foundation due to a known unbalance on the rotor. The key to this problem is the derivation of the forces exerted on the foundation at the bearings. Provided these forces can be derived, a variety of methods may be applied to extract the dynamic properties.

In this work therefore, the rotor is considered to be adequately modelled. It is assumed that the free-free modal properties of the complete rotor train is established from the models. It is worth noting that the free-free modes of the component rotors may be established experimentally.

CALCULATION OF BEARING FORCES

In this work therefore, the rotor is considered to be adequately modelled. It is assumed that the free-free modal properties of the complete rotor train is established from the models. It is worth noting that the free-free modes of the component rotors may be established experimentally. At any point x along the rotor,the displacement y is given by

$$y(x) = \int_0^L G(x,x')\,F(x')\,dx' \qquad (1)$$

where F(x') represents the force per unit length along the rotor, and G(x,x') is the Greens function of the rotor, representing the response at point x arising from a unit force at x'. This function is dependant on frequency , and using the standard result

$$G(x,x') = \sum \frac{\psi^{*}{}_{n}(x)\,\psi_{n}(x')}{\omega^{2} - \omega_{n}^{2}} \qquad (2)$$

where the modes shape have been normalised to the rotor mass, i.e.

$$\int_0^L \psi^{*n}(x)\rho(x)\psi_n(x)dx=1 \qquad (3)$$

where $\rho(x)$ is the mass per unit length of the rotor at x.

In the above equation, no allowance has been made for damping within the rotor. There would be little difficulty in including such a term but in practice, damping from the bearings and supporting structure will normally be dominant in turbo machinery. In the present calculation the damping is neglected for the sake of clarity.

The forces acting on the rotor are of two types, the unbalance at various locations which are acting at location x_e, and the unknown bearing reaction forces acting at the locations $x_{b1},..x_{bn}$. It is assumed that the rotor unbalance is known. This may be achieved in practice by analyzing the differences in response of subsequent balancing runs of the machine. The bearing forces $F_{b1}..F_{bn}$ have yet to be determined. At each of the bearings of the system, the force can be related to the shaft displacement within the bearings.

Writing the displacements of the shaft and bearing pedestal by y_s and y_p respectively, combining equations 1 and 4 gives an expression for the displacement of the shaft at any point x

$$y(x)=G(\omega,x,x_e)m\omega^2 e+\sum k_n(y_s(x_n)-y_p(x_n))G(\omega,x,x_n) \qquad (4)$$

n being summed over all bearings. Given measured values of the pedestal displacements $y_p(x_n)$, then a set of simultaneous equations may be formed for the shaft displacements at the bearing location by setting $x= x_n$. Hence

$$y(x_m)=G(\omega,x_m,x_e)m\omega^2 e+\sum k_n(y_s(x_n)-y_p(x_n))G(\omega,x_m,x_n) \qquad (5)$$

Thus, on determining the parameters y_s the forces acting on each of the bearing pedestals can be determined. Note that the parameter y may be a vector. Having established the forces acting on the foundation due to the rotor, the forces and bearing responses may be used to identify the dynamic properties of the foundation structure.

SENSITIVITY TO BEARING UNCERTAINTY

As outlined above , a priori knowledge of the bearing properties is imprecise and hence there is a need to establish the corresponding uncertainty in the forces applied to the structure. To examine the sensitivity, we examine the case of a simple two bearing rotor, using the simplified notation $G_{ij} = G(\omega, x_i, x_j)$. The equations for the two bearing displacements become

$$y_{s1}=G_{1e}m\omega^2 e+G_{11}k_1(y_{p1}-y_{s1})+G_{12}k_2(y_{p2}-y_{s2}) \quad (6)$$

and

$$y_{s2}=G_{2e}m\omega^2 e+G_{21}k_1(y_{p1}-y_{s1})+G_{22}k_2(y_{p2}-y_{s2}) \quad (7)$$

In these equations the pedestal motion y_p is measured, and hence the shaft motion is readily calculated in terms of the bearing stiffness coefficients k_m. These equations involve the inversion of a matrix A defined as

$$A=\begin{matrix}1+G_{11}k_1 & G_{12}k_2\\ G_{12}k_1 & 1+G_{22}k_2\end{matrix} \quad (8)$$

Although the motion is clearly very dependent on the values of k_m, the values of force are much less sensitive to the values of bearing stiffness. This may be examined by differentiation with respect to k. After some algebra it may be shown that ,

$$(y_{sj}-y_{pj})(k_j+G_{jj}^{-1})=C_j \quad (9)$$

for bearing j.
Alternatively, if the shaft motion y_s is measured, the analysis of the bearing forces is rather simpler, for in this case, it is easily shown that

$$\begin{matrix}F_1\\ F_2\end{matrix}=G^{-1}\begin{matrix}G_{1e}m\omega^2-y_{s1}\\ G_{2e}m\omega^2-y_{s2}\end{matrix} \quad (10)$$

where G is the matrix formed by the components of the Greens function for the free-free rotor.

The analysis has been tested by reference to a rigid rotor mounted on two bearings and results will be presented for this case. From the nature of equation 10, it is readily seen that provided the rotor motion at the bearing location is measured, the forces only become indeterminate at the free-free critical speeds. Note however, that these modes are of no particular practical significance.

For practical reasons it is attractive to derive the forces without a measurement of absolute shaft motion. Equation 10 shows that in this case the forces arising at the bearing are only sensitive to bearing stiffness in cases where the bearing stiffness is not significantly greater than that of the foundation. This fact has some important practical implications for research in the motion of rotating machinery.

THE GPT METHODOLOGY. NEW FIELDS OF APPLICATION

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SUMMARY

As well known, a distinctive feature of heuristically based generalized perturbation theory (GPT) [1] methodology consists in the systematic use of importance conservation concepts. This function is uniquely defined in relation to a given system response , for example, a neutron dose, the quantity of plutonium in the core at end of cycle, the temperature of the outlet coolant.

The GPT method was first derived in relation to the linear neutron density field. Then it was extended to other linear, or linearized ones. For all these fields the equation governing the importance, or weight function was defined, associated with a response of interest, generally defined as

$$Q = \int_{t_0}^{t_F} < \mathbf{h}^+, \mathbf{f} > dt \equiv << \mathbf{h}^+, \mathbf{f} >> ,$$

with $\mathbf{h}^+$ given and $\mathbf{f}$ being the function describing the field of interest. Weighting the source terms ($\mathbf{h}$) of the governing linear, or linearized equations with the importance function ($\mathbf{f}^*$) gives the important reciprocity relationship

$$<<\mathbf{f}^*, \mathbf{h}>> \equiv Q = <<\mathbf{h}^+, \mathbf{f}>>$$

on which the GPT methodology is based.

Consider now a generally nonlinear physical model defined by a number of parameters p_j (j=1,2,...,J) and described by an N-component vector field $\mathbf{f}$ obeying equation

$$\mathbf{m}(\mathbf{f}|\mathbf{p}) = \mathbf{0} .$$

vector $\mathbf{p}$ representing the set of independent parameters p_i fully describing the system.

Along the GPT methodology the sensitivity coefficient s_j ($\equiv \frac{dQ}{dp_j}$) is given by expression (assuming $\mathbf{h}^+$ is independent of p_j)

$$s_j = <<\mathbf{f}^*, \frac{\partial \mathbf{m}}{\partial p_j}>> ,$$

where the importance f^* obeys equation

$$H^* f^* + h^+ = 0 \ ,$$

H^* being the adjoint of the Jacobian of the governing system.

The GPT methodology has been widely applied to the first two fields. We shall limit here description to its potential use.

As a starting problem to test the potentiality of the GPT methodology in radionuclide particle migration problems, a zero dimension model describing the solution mining for salt consumption [2] has been considered. A unique cavity is created by dissolution in a bedded salt formation where radioactive waste disposal is located. During the cavity formation, waste packages are degraded, brine is contaminated and radionuclides in solution lead to a salt contamination. The exposure due to ingestion of cantaminants is estimated.

The equations used for the direct calculations, on which basing for the GPT methodology, are the following:

1. Sal concentration (c) in the brine evolution equation

$$\frac{dc}{dt} = \frac{(1-c)\rho_{salt}\frac{dV}{dt}}{(1-\alpha f)V\rho_b} - \frac{c\rho_w q_w}{\rho_b V 1-\alpha f)}$$

where:

ρ_{salt} , ρ_b , ρ_w are salt, brine, water volumetric masses, respectively;
V is the cavity volume;
q_w is the water injection rate;
α is the insoluble rate;
f is the swelling coefficinet.

It is also

$$\rho_b = \rho_w + c\frac{\rho sat - \rho_w}{c_{sat}} \ .$$

where c_{sat} is the salt concentration in the brine at saturation and ρ_{sat} is the brine density at saturation.

2. Cavity volume (V) and insoluble hight (H_i) evolution equations

$$\frac{dV}{dt} = 2\pi R H \frac{dR}{dt} - \pi R_c^2 \frac{H_i^2}{H_c^2}\frac{dH_i}{dt} \ .$$

(R_c and H_c are the radius and the height of the cavity, respectively)

$$\frac{dH_i}{dt} = 2\,\alpha\, f\, H\, \frac{H_c^2}{H_i^2}\,\frac{R}{R_c^2}\,\frac{dR}{dt} \quad .$$

3. Dissolution kinetic equation

$$\frac{dR}{dt} = A(\rho_{sat}\, c_{sat} - \rho_b\, c)^{5/4}\left[1{,}7 + \frac{0.26}{58.5}(\rho_{sat}\, c_{sat} - \rho_b\, c)\right]$$

$$(A=1.07\times10^{-4}\ ,\ c_{sat}=0.26\ ,\ M_{NaCl}=58.5)$$

4. Salt production evolution

$$P_{salt} = \rho_{salt}(1-\alpha)\,\frac{dV}{dt} - (1-\alpha f)\,\frac{d}{dt}(\rho_b V c).$$

5. Activity evolution within the cavity

$$\frac{dM_i}{dt} = A_i\,\tau\, S - \frac{q_b\, M_i}{V}$$

where

A_i is the activity per mass unit of ith waste nuclide;
τ is the leaching rate of glass matrix (g/cm^2 day);
S is the exposed surface;
q_b is the brine outflow rate $\left(= \frac{P_{salt}}{\rho_b\, c}\right)$.

6. Activity per salt mass unit extracted

$$\alpha_i(t) = \frac{q_b(t)\ M_i(t)}{V(t)\ P_{salt}(t)}$$

As response the individual individual dose rate at time t_F from a given i'th radionuclide was considered

$$D = \alpha_i(t_F)\,\Lambda\, F_i \equiv \int_0^{t_F} \alpha_i(t)\,\Lambda\, F_i\,\delta(t-t_F)\,dt \quad ,$$

Λ and F_i being the annual salt consumption per person and the dose factor for the i-th radionuclide, respectively.

Denoting variables c, V, R, P_{sel}, M_i, α_i with f_1, ..., f_6, respectively, following the lines of the GPT methodology, the equations relevant to the importance functions f_1^*, ...,f_6^* have been defined. Sensitivity coefficients of the response relative to parameter changes have been then calculated , which allowed to identify the most important among them. Comparison with analogous response changes obtained by direct calculation demonstrates the validity of the methodology.

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[1] A. Gandini, "Generalized Perturbation Theory Methods. A Heuristic Approach", Advances in Nuclear Sci. and Techn., Vol 19, J. Lewins and M. Becker Eds., Plenum Press, New York, (1987) p 205.
[2] EVEREST Project report, Vol III (Salt Formations), CEC report (in preparation).

THE EFFECT OF CORRELATED VARIABLES ON A ONE–WAY SENSITIVITY ANALYSIS

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One–way sensitivity analysis measures a variable's influence by observing the output while varying one and only one variable at a time. Judging by the ubiquitous presence of one-way sensitivity analysis in the decision analysis literature and in the software programs (DPL, Supertree, @Risk, *etc*), it appears to be the choice of most analysts in determining the influence of each variable. Clearly, holding all variables fixed except one ignores any correlation between the existing variables. Ignoring the dependence structure could result in a compromised sensitivity analysis. For example, if there exists a nonzero dependency among the judgements, then it is possible to misspecify influential variables either by missing influential ones or giving undue weight to spurious ones.

Reilly [1] proposes a procedure to incorporate the dependency relations, called dependent sensitivity analysis (DSA). In this short note, DSA is applied to an example adopted from Clemen [2] that demonstrates how DSA enhances a one–way sensitivity analysis by conveying insights not available through the traditional analysis.

To incorporate the dependency relations, DSA uses a symmetric positive-definite matrix whose entries are pairwise measures of dependence. The dependency matrix generates a linear transformation that is then used to transform the original set of variables into a new set of variables that are orthogonal with respect to the metric defined by the dependency matrix. Existing sensitivity analyses' techniques are then applied to the orthogonal transformed variables. The proposed procedure does not replace any existing sensitivity analyses; rather it gives the decision analyst the freedom to model and utilize dependency relations among the input variables when using existing techniques.

Eagle Airline's Example

Dick Carothers, the owner of Eagle Airlines, wishes to decide whether to invest his profits of \$52,500 in a money market or to expand his fleet with the purchase of a Piper Seneca. He has been wishing to expand for the last few years, but he is not sure if this is the appropriate time. His decision criterion is whether the new plane will generate more profit than the money market alternative. Table 1 gives the range for each of the variables Carothers has determined to be relevant to this decision and his base values. The criterion function for this problem is the profit expected from purchasing the plane minus \$4,200, which is the amount Carothers feels he can earn from investing his \$52,500 in the money market.

From a standard sensitivity analysis (assuming all the input variables are uncorrelated), we have that the variables Capacity on Flights, Operating Cost, Hours Flown and Price Level/Hour could significantly affect Carothers' decision to purchase the plane (When $f(X) = 0$, then Profit = \$4,200). The sensitivity analysis indicates that profit would be substantially lower if the Price Level/Hour dropped from \$100 to \$95 per person per hour. The boundary value of Price Level at which Carothers would invest instead of purchase the plane, called the critical or threshold value, is \$97.50. The standard analysis assumes that a higher price has no effect on Capacity. We suspect, though, that as price increases, the quantity demanded will decrease. Standard sensitivity analysis ignores any dependency relations and thus has no way to compensate for this trade–off.

Table 1 Range of Input Values

Variable	Low	Base	High
Ratio of Charter Fights	40%	50%	60%
Capacity	40%	50%	60%
Price Level	\$95	\$100	\$108
Hours Flown	500	800	1000
Operating Costs	\$230	\$245	\$260
Percentage Financed	40%	50%	60%
Interest Rate	10.5%	11%	13%
Purchase Price	\$85,000	\$87,500	\$90,000
Insurance	\$18,000	\$20,000	\$25,000

To determine the effects of variables simultaneously covarying according to pairwise correlations, we use the correlation matrix:

	Hours	*PriceL*	*Cap*	*Ratio*	*OpCost*	*Insur*	*%Fin*	*Inter*	*PurPr.*
Hours	1.0								
PriceL	−.5	1.0							
Cap	.5	−.25	1.0						
Ratio	.25	.25	−.25	1.0					
OpCost	0	0	.25	.25	1.0				
Insur	.25	0	0	0	0	1.0			
%Fin	0	0	0	0	.25	.25	1.0		
Inter	0	0	0	0	0	0	−.5	1.0	
PurPr.	0	0	0	0	0	0	.75	−.25	1.0

Using the eigenvectors of **R**, a linear transformation **L** is generated that transforms the uncorrelated X-variables into a set of uncorrelated Y-variables. The Y-variables are affine combinations of the X-variables. In this case,

$$Y_2 = -.60Hours + .52PriceL - .53Cap + .10Ratio - .08OpCost - .13Insur + .14\%Fin - .12Inter + .16PurPr. \quad (1)$$

Therefore the variable Y_2 is a contrast between Price Level on one hand and Hours Flown and Capacity on the other hand, because the coefficient of Price Level is positive (.52) and the coefficients of Hours Flown and Capacity are negative (-.60 and -.53). When interpreting Y_2, the other X–variables in the Y_2 factor are ignored due to their relatively small loadings, and thus low correlation with Y_2. Clearly, Y_2 is a Price/Demand factor with Price being measured by Price Level and Demand being measured by Hours Flown and Capacity. As the Y_2 factor increases, then Price will be increasing while Hours Flown and Capacity will be simultaneously decreasing. Thus, this factor automatically tracks the trade–offs between price and demand that are encoded in the given matrix of dependencies.

Next, a one-way sensitivity analysis using the uncorrelated Y-variables as the input variables is run. The results indicate that there are two factors, Y_2 and Y_7, that drop the profit below the minimum acceptable value of \$4,200. The Y_2 factor is considered influential because for the values Carothers has determined probable, the profit could dip below the minimum \$4,200. Solving $f(Y_2^*) = 0$, we find $Y_2^* = 1.637$. Hence, the critical values for

the original input variables are: Price Level = \$102.74; Hours Flown = 678 hours; and Capacity = 45.64%.

Insights not available using traditional sensitivity analysis are now evident from the above critical values. The traditional analysis indicated that only too low a Price Level (below \$97.50) would drop profit below the \$4,200 benchmark. The analysis above, however, indicates that a Price Level too high could also drop the profit below \$4,200. In particular, if the Price Level rises above \$102.74, Carothers should expect Hours Flown and Capacity to drop sufficiently low so that his profit would fall below the established \$4,200. Hence, by incorporating the dependency relations, we have discovered that too high a price could have an adverse effect.

The component Y_7 is also a contrast, this time between Operating Cost and the variables Price Level and Capacity. For negative values of Y_7, the profit will be below the \$4,200 minimum. As Y_7 increases, so will the profit. The interpretation is that as Price Level and Capacity increase while Operating Cost decreases, profit will increases. This is intuitively obvious. Thus Carothers must monitor these variables or perhaps stochastically model them in subsequent analysis because they can significantly alter the profitability of the airline. The critical values are: Price Level = \$99.11, Capacity = 48.88%, and Operating cost =\$246.12. Table 2 summarizes the results from the two analysis.

Table 2 Influential Variables and Critical Values

Traditional	Utilizing Dependence
Price Level (\$97.50)	Price Level (\$102.74)
	&
Operating Costs(\$252)	Hours Flown, Capacity
	(678 hours, 45.6%)
Hours Flown(664 hours)	
	Operating Costs(\$246)
Capacity (47%)	&
	Price Level, Capacity
	(\$99.11, 49%)

Table 2 indicates that Price Level must stay between \$99.11 and \$102.74 for the purchase of the plane to be the alternative ranked first. It is clear from Table 2 that DSA identifies groups as well as individual variables as influential. The groups are actually linear combinations of the individual variables. Additional insights into the nature of the influence can be inferred from both the magnitude and direction of the coefficients. It is often the case that the linear combination itself has a meaningful interpretation. For example, Y_2 could be interpreted as a Price/Demand factor and Y_7 as a Cost/Revenue factor. DSA provides the DA more flexibility and information when presenting to Carothers the influential variables in the decision since the DA can not only detail the influence and critical values of the variables individually, but can also explain the role of the influential factors in the decision. DSA presents additional opportunities to think creatively about the decision.

References

[1] Reilly, T. 1995. Sensitivtiy Analysis for Dependent Variables. Submitted to *Management Science.*

[2] Clemen, R. T. 1991. *Making Hard Decisions: An Introduction to Decision Analysis.* PWS–Kent, Boston, MA.

LOCATING SENSITIVE REGIONS BY LEARNING FROM SIMULATION DATA

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1 Introduction

Sensitivity Analysis (SA) is an important task when using modeling and simulation. Simulation of a model can be seen as evaluation of a blackbox function f_{model}, mapping n model factors $x_1, \cdots, x_n$ to m output values $y_1, \cdots, y_m$. The main task of SA is now defined as finding sensitivity coefficients:

$$S_{i,j} = \partial y_i / \partial x_j \text{ (or } S_{i,j} = \Delta y_i / \Delta x_j \text{, if differentiation is not possible.)} \quad (1)$$

Existing approaches to obtain information about the sensitivity of a model can be categorized into different approaches:

- **model based**: the model is described by a function.
  E.g. Blake et.al. [1] uses Markov Reward Processes for performance analysis of models. The reward measure is explicitly defined as a function of process states. In order to find sensitivity coefficients a linear system of derivatives of the reward measure in each state is solved.
- **simulation based**: sensitivity is estimated directly while simulation is running.
  For example the score function method can be used to analyze the model behaviour due to its sensitivity during one simulation run [6].
- **data based**: the model function f_{model} is approximated based on simulation data.
  Kleijnen [4] takes into account some apriori knowledge about the model behaviour to design an extended regression function f_{approx} that approximates f_{model}, representing the model behaviour. Simulation data is used to compute the parameters of the function f_{approx}.

Comparing these categories the main advantage of data-based approaches is their usability for different simulation models independent from the underlying modeling concept (e.g. queueing networks). Existing concepts (see for example [4]) are often based on some assumptions about the model behaviour, e.g. that f_{model} is a linear function of all factors. The resulting approximation function f_{approx} then can be differentiated and sensitivity can be computed directly. In complex models often these assumptions are not fulfilled. On the other hand, qualitative information about specific regions where factors are sensitive also helps to understand the model. In this paper we present a new data-based approach that is able to locate sensitivity regions. A rule generating algorithm from the Machine Learning Area is used and easy to interpret if-then-rules are derived from given data examples, in our case from simulation data.

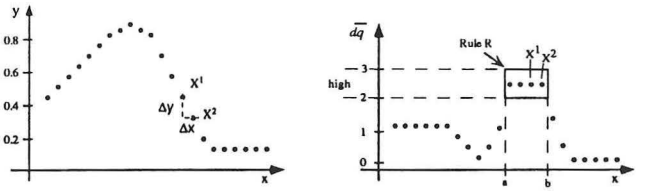

Figure 1: *Left*: A one-dimensional example of sampled points and the differences Δx and Δy between $\vec{x}^1$ and $\vec{x}^2$ are shown. *Right*: The corresponding values of $\overline{dq}$ are illustrated. The class *high* covers the interval $[2 \cdots 3]$ so the generated rule R: "if $(a \leq x \leq b)$ then class *high*" describes the region $[a \cdots b]$ of x where sensitivity stays within this interval.

2 Locating Sensitive Regions with Learning

The main idea of this approach is to use a rule learning algorithm to extract knowledge about the model behaviour based on data from simulation experiments. The resulting rules describe regions where the model tends to be more or less sensitive. In [7] we have used a rule learning algorithm to find regions of *insensitivity*. In contrast, the method described in this paper uses a specific preprocessing of the simulation data before rule learning. This leads to rules that describe regions of *sensitivity*. The approach consists of three steps: data generation, computation of difference quotients and finally learning sensitive regions.

- First, a full factorial design is used to plan a number of experiments and to **perform simulation runs**. After performing simulation runs with different factor combinations one interesting output parameter y is selected for further sensitivity investigation. Each simulation run is represented as one point $(x_1, \cdots, x_n, y)$ in a $(n+1)$–dimensional factor space, when n factors are given.
- The next step is the **computation of difference quotients**. For each point $\vec{x} = (x_1, \cdots, x_n)$ a set of adjacent points (e.g. the nearest neighbour in each direction of the factor space) is taken and the difference quotient $dq = \Delta y / \Delta x$ between the two points is computed:

$$dq(P^1, P^2) = \frac{\Delta y}{\Delta x} = \frac{|y^1 - y^2|}{|\vec{x}^1 - \vec{x}^2|}, \text{ with } P^i = (\vec{x}^i, y) \text{ and } \vec{x}^i = (x_1^i, \cdots, x_n^i) \tag{2}$$

  Here, Δx represents the Euclidean Distance between the points in a normalized parameter space and Δy the difference between the output values. On the left side of figure 1 an example is shown. For each point the average of the absolute values of difference quotients considering all adjacent points is computed. The resulting data $(x_1..x_n, \overline{dq})$ describes the sensitivity of each point.
- The last step, **learning sensitive regions**, includes a quantization of the output $\overline{dq}$ into k nonoverlapping intervals (represented by k classes). For learning regions of sensitivity RecBFNs (Rectangular Basis Function Networks) are used. The efficient learning algorithm of RecBFNs uses a set of classified data examples as input and constructs a set of hyperrectangles in the parameter space (for details see [2]). Each hyperrectangle is assigned a class and can be easily represented as a rule like:

$$\text{if } (a_1 \leq x_1 \leq b_1) \text{ and .. and } (a_n \leq x_n \leq b_n) \text{ then class } C. \tag{3}$$

  A rule describes restrictions on attributes and corresponds with only one class. To find meaningful rules quantization of the continuous values $\overline{dq}$ is difficult because simulation data tends to be very noisy due to its underlying stochastic process. Two extensions to RecBFNs are being used to deal with these problems. A compatibility relation between classes was introduced. This leads to a more robust construction of rules with a controllable tolerance towards noise. Furthermore, an additional fuzzyfication module allows to build not only a classifier but also a fuzzy graph, which

can be used as a function approximator (the concept of building fuzzy graphs is described in [3]). One possible usage is to calculate sensitivity for unknown points. That means to use the rules as a metamodel (see also [5]) but in this paper our focus is the analysis of the resulting rules[1].

Using RecBFN with data about difference quotients result in rules that describe regions for each factor, where the sensitivity stays within the range represented by the class. High values of $\overline{dq}$ mean that little changes in factors causes high changes in the output. An example of a rule is shown on the right side of figure 1. In regions of low sensitivity the model seems to behave uncritical, while in regions of high sensitivity a more detailed investigation may be useful. A high sensitivity level can be caused by strong increase, strong decrease, or by steep optima. To distinguish these situations, an additional analysis of such sensitivity rules in combination with insensitivity rules [7] seems to be an interesting focus in future.

In the paper an example of a complex queueing network model will be used to demonstrate how the approach works in practice.

3 Conclusions

The presented approach generates rules that describe regions of sensitivity. The approach is easy to handle and efficient because rule generation with RecBFNs is done automatically. An additional advantage is that no assumptions about the model function f_{model} have to be made apriori. Since rule learning depends on the simulation data, quantity and quality of the data directly influence the results. For a detailed sensitivity analysis it is possible to start with this approach to locate regions of sensitivity followed by the application of a more accurate method focusing on regions of interest.

4 Acknowledgements

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References

[1] Blake, J. T.; A. L. Reibman and K. S. Trivedi: "Sensitivity Analysis of Reliability and Perfomability Measures for Multiprocessor Systems" in Proc. of the ACM Sigmetrics Int. Conference on Measurement and Modelling of Computer Systems, Santa Fe, New mexico, pp. 177-186, 1988.

[2] Berthold, M. R. and K.-P. Huber: "From Radial to Rectangular Basis Functions – A New Approach for Rule Learning from Large Datasets", Internal Report of the University of Karlsruhe 15/95, 1995.

[3] Berthold, M. R. and K.-P. Huber: "Neural Network based Construction of Fuzzy Graphs", in Proc. of the Fourth Annual Conference on Fuzzy Theory and Technology, North Carolina, 28.-30.9.95, (to appear), 1995.

[4] Kleijnen, J. P. C.; G. van Ham and J. Rotmans: ' "Techniques for Sensitivity Analysis of Simulation Models: A Case Study of the Greenhouse Effect" in Simulation, 58, 6, pp. 410-417, 1992.

[5] Pierreval, H.: "Rule-based simulation metamodels", European Journal of Operational Research, 61, pp. 6-17, 1992.

[6] Rubinstein, R. and A. Shapiro: "Discrete Event Systems: Sensitivity analysis and stochastic optimization by the score function method", Chichester, Wiley, XV, 1993.

[7] Huber, K.-P. and H. Szczerbicka: "Sensitivity Analysis of Simulation Models with Decision Tree Algorithms" in Proc. of the European Simulation Symposium ESS'94,Vol.1, pp. 43-47, 1994.

[1] The approximation error could be used as an indicator for the quality of the rule base.

SENSITIVITY ANALYSIS OF RESULTS TO VARIATION IN THE SAMPLING ERROR IN THE CONTEXT OF REPEATED SAMPLE SURVEYS

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1. Introduction

When surveys with similar data items are conducted on repeated occasions certain estimation and data analysis methods are available which are non possible with single occasions surveys. For example, efficient estimation methods for the current occasion can depend on data previous occasions. This occurs when there are overlapping sampling units between occasions and, hence, the survey errors can be correlated over time. As well, the series of estimates from a repeated survey are often modelled by the data users. A common example of this is to assume an autoregressive-moving average (ARMA) model. However, most existing procedures for estimating the unknown parameters of this model assume that the input data are not subject to survey error.

In this paper we show a procedure for estimating these model parameters when the data contain survey errors. The covariance structure of the survey errors we consider include some cases where the survey errors are correlated over time.

2. The model

The model is based on the use of signal extraction results from time series analysis to improve estimates in repeated surveys (Bell and Hillmer, 1990). In this framework, the observed survey estimate for time t (t=1,...,T), g_t , is represented as the sum of two independent processes, the true population value (*signal*), θ_t , and the sampling error (*noise*), ε_t,

$$g_t = \theta_t + \varepsilon_t . \qquad (1)$$

Given a model for θ_t and design-based information on the covariance structure of ε_t, the observed sample series may be decomposed into its *signal* and *noise* components. The basic approach of this paper is to represent the signal and the noise as an ARMA model (Binder and Dick, 1990).

We first describe an integrated seasonal autoregressive-moving average model for θ_t. We let L be the backshift operator; $\nabla = 1 - L$ and $\nabla_s = 1 - L^s$, where s is the seasonal period. We define the following polynomial functions: $\varphi(L)$, $\lambda(L)$, $\omega(L)$ and $\mu(L)$, respectively with p, P, q, and Q degrees.

The seasonal ARIMA (p,d,q) $(P, D, Q)_s$ model for $\{\theta_t\}$ is given by

$$\lambda(L^s)\ \varphi(L)\ \nabla^d\ \nabla_s^D\ \theta_t = \mu(L^s)\ \omega(L) b_t \qquad (2)$$

where the b_t' s are independent $N(O, \sigma_b^2)$.

We now consider the sampling errors $\{\varepsilon_t\}$ of expression (1). This component represents errors that arises from sampling only a portion of the total population. Its structure depends upon the survey design, the form of estimator and population characteristics. Our analysis will focus the attention on the major sources of heteroscedasticity and autocorrelation of sampling error. To capture the autocorrelated and heteroscedastic structure of ε_t, in this paper we assume that the sample error process is given by:

$$\varepsilon_t = k_t\ e_t \qquad (3)$$

with e_t reflecting the autocovariance structure, assumed to follow an ARMA (m, n) process given by

$$\phi(L) e_t = \psi(L) c_t \qquad (4)$$

where: $\phi(L)$ and $\psi(L)$ are polinomial functions with m and n degrees and c_t's are independent $N(0, \sigma_c^2)$, the factor k_t represents the changing variance over time and it is expressed by:

$$k_t = \left(\sigma_{\varepsilon_t}^2 / \sigma_e^2\right)^{1/2} \qquad (5)$$

being $\sigma_{\varepsilon_t}^2$ and σ_e^2 are respectively the variance of ε_t and of e.

For estimation and signal extraction, the component signal and noise models are put in state-space form. The signal and noise are the *state variables,* $\underline{z}_t$, whose evolution over time is described by the transition equation

$$\underline{z}_t = \underline{F}\underline{z}_{t-1} + \underline{G}\underline{v}_t \qquad (6)$$

and the state variables are transformed into the observed sample series, g_t, by the observation equation

$$g_t = \underline{H}_t^{'} \underline{z}_t \qquad (7)$$

where: $\underline{F}$ is a fixed transition matrix; $\underline{G}$ is a fixed matrix, $\underline{v}_t$ are independent random disturbances and $\underline{H}_t$ is a fixed matrix.

The Kalman filter produces an estimate of the signal θ_t which is optimal with respect to the model assumptions and from the point of view of survey sampling is also a design-consistent estimator (Anderson and Moore, 1979).

3. Sensitivity analysis

As an illustrative example of the above described model we analyse time series of employment, which are estimated in the italian Labour Force Survey (LFS).

The LFS is a nationwide quaterly survey designed to produce estimates of the labour force status of the population, at national and regional level.

Here we focus on sensitivity of results to variations in the sampling error model, since this is the derminated with less information than the signal model. Our approach is to vary parameters of the sampling error model, than reestimate the signal model and redo the signal extraction. While it would be preferrable to have more formal statistical measures of the signal extraction error due to model error, this approach should at least help indicate in what rescpect the signal extraction results are sensitive to parameter variation and in what respect they are not.

REFERENCES

[1] BELL, W. R., HILLMER, S. C. (1990) " The Time Series Approach to Estimation For Repeated Surveys", Survey Methodology, Vol. 16, Statistics Canada.

[2] BINDER, D. A.., DICK, J. P. (1990) "A Method for the Analysis of Seasonal ARIMA Models", Survey Methodology, Vol. 16, Statistics Canada.

[3] ANDERSON, B. D. O., MOORE, J. B. (1979), "Optimal Filtering", Prentice Hall, New York.

SENSITIVITY ANALYSIS IN THE SPACE-TIME STATISTICAL MODELS

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1) Statment of the problem

A space-time model on a domain D can be formulated as a system of differential equations. Sometime such equations can be non-linear and the statistical fluctuations in the estimate parameters can induce large deviation in the outputs. The sensitivity analysis of the system is a very important tool in the control of system response to parameters variation. We describe, now, the statistical estimation problem and the system building methods.

The domain D is partitioned in N sub-domains D_i, ($\bigcup_{i=1}^{N} D_i=D$; $\bigcap_{i=1}^{N} D_i=\emptyset$) , for each sub-domain a stochastic process $Y_i(t)$ is defined. The available data concerns n domines (or sites) for a time interval (0,t) and n<N. The problem is to predict the values of Y on the set of unobserved sites and forecasts new values, overall the sites of D, for a given time interval (forecast orizont).

D is an irregular lattice (ordered discrete set of sites) the conditional probability $F(y_i|y_j)$ of the random process on each point i , ($i \notin s$) given the variable in the points s=(1,2,...n) becomes:

$$F(y_i|y_j\ ;j \in s)=\exp(-(\alpha_i y_i+\sum_j \beta_{ij} y_j)/(1+\exp(-(\alpha_i y_i+ \sum_j \beta_{ij} y_j)) \quad ; \quad i \in (D\backslash s),\ j \in s \quad (1)$$

The time dependence can be expressed as:

$$A(t)=GA(t-\Delta t)+HZ(t) \qquad (2)$$

In (1) and (2) the y_i and y_j indicates the process at points i and j , $F(y_i|y_j)$ is the probability of the random variable (experimental results) at point i given the results at points $j \in s$; under particular conditions, (1) is known as the Ising model (from Statistical Mechanics). In the equation (2) A(t), is the parameters vector $\alpha(t)$ and $\beta(t)$. The matrix G contens the autoregressive parameters for the vectorial process A(t) and H is the parameters matrix of the vectorial noise Z(t). G and H has to be estimated from available data (time series) . The model (2) is known as VARMA (Vectorial AutoRegressive Moving Average) and it is linked to model (1) as predictor of future parameter values for the model (1).

2) The model for a pattern of points on D

The model (1) has only the hipothesis that Y is binomial. We indicate with Λ the n realizations of this variable on D (it is a " pattern ") in a given time t. Let us indicate μ and η be some pre-defined measure on D and with y the set of conditional variables , the potential of such pattern can be defined as (Preston 1974):

$$\Psi(\Lambda)=-\ln[\mu(\Lambda)/\mu(\emptyset)] \tag{3}$$

bat $\mu(\emptyset)=[1-\mu(y)]^n$ and $\mu[\Lambda]=\mu(y)^{\eta(D)}[1-\mu(y)]^{n-\eta(D)}$; $y \in D$ (4)

from (3) and (4) we have:

$$\Psi(\Lambda)=-\ln[\mu(y)/(1-\mu(y))]^{\eta(D)} \tag{5}$$

then $$-[\Psi(\Lambda)/\eta(\Lambda)]=\ln[\mu(y)/(1-\mu(y))] \tag{6}$$

as $\eta(\Lambda)=1$:

$$\mu(y|\Lambda)=\exp-[\Psi(\Lambda)]/[1+\exp(-\Psi(\Lambda))] \tag{7}$$

If we expand the potential Ψ in term of interactive potential between couple of pionts (Besag 1974) we have:

$$\Psi(\Lambda)=\sum\sum\phi_{ij}(y_i,y_j) \tag{8}$$

Substituting (8) in (7) we have the model (1). The formula (7) can be used to build an estimator for the unobservd points of D. The variance of this estimator, based on spatial models, can be obtained from the general formula:

$$V(\Lambda)=V(y)+\sum_{i,j\in s}\sum\lambda_{ij}G(y_i,y_j)-2\sum_{i\in s,j\notin s}\sum\lambda_{ij}G(y_i,y_j) \tag{9}$$

(9) is an instrument for sensitivity analysis of the system. Infact it permit us to compute the probabilty of parameter ocillations (due to unobservable noise) near the instability points.

3) Sensitivity, Stability and Chaos

Many works, in the last time, are devoted to develope methodologies to analize the behaviours of

dinamical systems . The sistems of differential equations, describing the dinamics of phenomena, can be studied as systems response to input variations (stability) and as system response to parameters variation (sensitivity). In both the case (instability or great sensitivity) the system exibit chaotic behaviours.

In particolar, the equation (1) is unstable for $\alpha=0$ and $2.9<\beta<3.9$ (Nijkamp,Reggiani -1990) . Then, for etimated parameter near this interval, small fluctuation can produce outputs fluctuations that cannot be attributed to the imput fluctuations.

The proposed methodology to analize the system sensitivity, is based on the search for the stability (or fixed points) of the system (1) using Liapunov theory. To this purpose we can observe that the system (1) is the solution of the Bernoully differential equation:

$$dY_i=(\beta Y_i+\alpha Y_i^g)dt \quad ; \quad g=2 \quad , \quad i=1,2....n \tag{10}$$

Studing the orbits of this system it is possible, with Liapunov functions, to compute the stability points and the actractors. The sensitivity analysis can be pursuit with the variance function (9) in wich the function G is the spatial autocorrelation function near this points. For the model (2) sensitivity analysis can be conduced with standard methods on matrix G and H.

From the formula (9) it is olso possible to obtain the design-based variance for the expansion estimator under simple random sampling:

$$Y_i=(1/n)\sum_{j\in s} y_j \tag{33}$$

Then a comparative study of sensitivity of design based and model based approach to spatial estimation, will be pursuit.

REFERENCES

Aoki M. (1987) State space modelling of time series; *Springer verlag.*

Doob J.L. (1984), Classical Potential Theory and Its Probabilistic Counterpart. Springer Verlag.

Freedman,D.(1978) Markow Chains - Wiley.

Kendall M.G. and Moran P.A.P(1973) Geometrical Probability. *Griffin,s Statistical Monographs & Courses, London.*

Holevo A.S. (1982) Probabilistic andStatistical Aspects of Quantum Theory. North-Holland.

Lauritzen S.L. (1982) Statistical Models as Extremal families. Aalborg University Press. Alborg.

Lauritzen S.L. (1984) Extreme point models in Statistics. *Scandinavian Journal of Statistica,* 11, 65-91.

Nijkamp P.,Reggiani A., Theory of chaos:relevance for analysing Spatial Processes. *Spatial choices and Processes. Elsevier Science Publishers* (North-Holland) 1990.

THE SENSITIVITY OF COMPUTER SIMULATION EXPERIMENTS TO ERRORS IN INPUT DATA

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Computer simulation is a widely used method of evaluating the performance of systems subject to random variation. Such simulations, especially those modelling complex systems, almost always require random variables, generated from given probability distributions, as inputs. The resulting outputs of interest, that are obtained from the simulation, are thus sensitive to the assumptions made concerning the statistical properties of these random inputs. Despite this there has been relatively little consideration of how accuracy of simulation experiments is affected by errors in assumptions concerning these inputs.

In this paper we consider both a classical statistical approach and also a bootstrap approach. We assume that the stochastic inputs come from parametric families of distributions. This allows a two-stage approach to be made to the problem. In the first stage we can establish confidence regions for the unknown parameters defining the input distributions. We can then, in the second stage, assess how errors in estimating these input parameters propagate through the simulation and affect the simulation output. An important feature of the problem is that there are two sources of error: the error that occurs in the modelling of the input distributions, and the error arising from the chance variation inherent in the simulation itself. We show analytically that asymptotically, at least, the overall error can be decomposed into these two components, and consequently, that we can assess the two errors quite separately.

Bootstrap methods, like simulation experiments, also use sampling techniques to reconstruct the statistical distributions of quantities of interest. The use of bootstrap methods in simulations has not received much attention. We show that they provide a very powerful and convenient alternative to classical statistical techniques in assessing the sensitivity of simulation experiments to input error. It is necessary to account for the bootstrap variability as well as the simulation variability. In standard statistical applications, simulation variability is not present. We show how to optimally and efficiently modify the bootstrap method to take this additional variability into account.

We illustrate the applicability of the above methodology by consideration of delay analysis in a computer communication network. A computer communication network is a collection of sites (or nodes) at which reside computing facilities that communicate with each other via a set of links (or channels). We consider a N-node, M-channel system where channel i has capacity C_i bits per second. The N nodes refer to the computer sites where the messages (or packets) arrive. It is assumed that nodal processing times are constant with value K. Traffic enters the network from external sources forming a series of Poisson processes with means γ_{jk} messages per second for those messages originating at node j destined for node k. All data messages are assumed to have random length, determined by an exponential distribution with mean $1/\mu$. As traffic in the system also incorporates control traffic, the average length of all messages is $1/\mu'$. If λ_i is the average traffic flow and P_i is the propagation time for a bit of information on channel i, then Kleinrock[1] has shown that, even for such a relatively realistic system, an analytic result is available for the average message delay, T, and is given by

$$T = K + \sum_{i=1}^{M} \frac{\lambda_i}{\gamma}\left[\frac{\lambda_i / \mu' C_i}{\mu' C_i - \lambda_i} + \frac{1}{\mu C_i} + P_i + K\right]$$

where

$$\gamma = \sum_{i=1}^{N}\sum_{j=1}^{M}\gamma_{ij}$$

The realism in such a system can be seen in the fact that such a model has been applied to the United States Department of Defense Advanced Research Projects Agency Network - ARPANET. We demonstrate the sensitivity of the model output to errors in the estimates for the numerous input variables

1 Kleinrock L, Queueing Systems Volume 2 : Computer Applications. John Wiley 1976

TESTING AND ASSESSMENT OF ENVIRONMENTAL MODELS

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Introduction

Sensitivity and uncertainty analyses in modelling contribute quantitative descriptions of the relative importances of individual parameters and processes, highlighting areas with significant contributions to the overall uncertainties of model predictions and giving markers for areas requiring substantial improvement (perhaps through directed experimental work). When modelling environmental systems, sensitivity and uncertainty analyses are often used in the assessment of the 'reliability' of the model and to provide uncertainty estimates on key model predictions.

A model of the dispersal of radioactive pollutants in the terrestrial or marine environment is typically composed of linked sub-models, representing processes understood to varying degrees. The sub-models may operate at quite different time and space scales, but all must inter-connect. For the model developer there will be choice of which processes to explicitly model and of how to parameterise the processes. Some parameters will be known more precisely than others; there may be conflicting evidence resulting in ranges for parameter values spanning several orders of magnitude while others will be tightly constrained. Some of the parameters may be time-dependent. Sensitivity analysis encourages investigations of the interactions between the various processes and is used to determine which processes should be further studied. Uncertainty analysis has a complementary role contributing in the final stages estimates of uncertainties on predictions. Taken together, the two methods contribute to the reliability assessment of the model; they provide tools when different models are being compared and when the models are used in predictive mode, the results may often be used to provide 'worst-case' calculations.

In this paper, the importance of sensitivity and uncertainty analyses will be discussed in developing, testing and assessing environmental models.

Model development

The purposes for which an environmental model is developed may vary, often it is developed for assessing the impact of some anthropogenic activity (eg impact of the accident at the Chernobyl nuclear power station or discharge of radioactivity from Sellafield waste processing plant). The required timescale for the predictions may span

minutes to thousands of years. The predictions may be required close to source (within a few tens of metres) or in the far-field (thousands of kilometres). It may in some circumstances be required to provide predictions for several different but linked media (eg seawater, sediment and fish). The model developer in sifting through existing knowledge already has performed some preliminary sensitivity and uncertainty analyses in selecting which processes to include.

In the development of the model, the modeller must work with an imperfect and incomplete description of the physical system. He must select features and processes to be parameterised, he must synthesise sometimes conflicting evidence, he must prioritise. In a number of recent international modelling studies (1,2,3), one objective has been to compare different model predictions ultimately with a view to contributing to assessment of model reliability. Each modeller was provided with the same basic information and the final end predictions compared. In this way, a preliminary sensitivity analysis based on model structure and modeller's interpretation has been performed. This is an often neglected, but important application of sensitivity analysis and interestingly the results have tended to show great sensitivity of results to modeller's interpretation. Model structure uncertainties may often be neglected, yet a fuller appreciation of them can only contribute to a more reliable decision tool (4). In such circumstances, where 'beliefs' are playing an important role, there is an opportunity for Bayesian methods to be developed and implemented, This will be discussed further.

Model parameterisations

Given the choice of parameterisations of specific processes, the assignment of parameter values and the propogation of the effect of parameter change is an area where the application of sensitivity analysis is well developed. There are many strategies for parameter selection and evaluation of the importance of pathways of pollutant dispersal. These will be mentioned only briefly. One end product of the sensitivity analysis is the ranking of the various processes or parameters, again a Bayesian approach would allow the incorporation of a-priori beliefs concerning the relative importance of each process. It would in certain circumstances allow the modeller's knowledge and experience to be included in the modelling process. Some suggestions as to how this may be performed and possible models will be presented,

Model testing and assessment

If we have as objective the development of a *realistic* and *reliable* model, then the model must be tested and assessed. Realism is not necessarily a primary goal in statistical modelling (pragmatism or the simplest model which satisfactorily satisfies the objectives is usually preferred), but in environmental modelling, one goal may be simply a descritpion

of the system and the model is simply a tool for visualisation. Reliability is a multi-dimensional concept (5) which includes understanding sub-model interactions, validation against observation (where possible), assessment of the effect of change in parameter values, and estimates of uncertainties of predictions. The uncertainties may be evaluated from a formal uncertainty analysis within a model, but may also be assessed from comparison of predictions between models. Appropriate endpoints which are both temporally and spatially discriminating of the model outputs must be selected.

It is clear that there will generally be no single *best* description of the environmental system (we lack the necessary information to define the complete system) and so in our assessment of the reliability of the predictions we must take into account the differeing interpretations (reflected in the different model structures) and the different sub-model parameterisations and their uncertainties. These general points will be covered in more detail and illustrated using a number of case studies.

References

(1) IAEA-VAMP project reports,

(2) BIOMOVS II technical report 3, March 1993.

(3) IAEA-IASAP project, Vienna, 1995.

(4) Draper D, 1995 Assessment and propagation of model uncertainty, JRSS(B), 57(1), 45-99.

(5) IAEA Safety Series, no 100, 1989. Evaluating the reliability of predictions made using emvironmental transfer models.

APPLICATION OF FAST TO A CLOSED ECOSYSTEM MODEL

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Ecosystem models are becoming increasingly important to understand and predict the impact of human actions on the world. These models contain a large number of parameters that are uncertain because they represent the response of living organisms to their surroundings. The uncertainty increases when biota must be grouped into a single compartment. In a closed system, the behavior of one compartment is quickly felt by the rest of the system which has the effect of coupling parameters. This set up strains any attempt to have confidence in the response of the model without a reasonable understanding of the parametric sensitivity. Furthermore, this knowledge is essential to focus research on the critical aspects of the environmental questions.

A computer model of a materially-closed marine microcosm has been developed. The model simulates 1-L microcosms, containing biota from anchialine pools in the Hawaiian Islands, that can sustain a constant population of shrimp for years. The stability of the systems depends on the initial number of shrimp and, once stable, the shrimp do not moult or reproduce. The model is an initial step in the investigation of endogenous control systems responsible for the stability of homeostatic ecosystems and was developed as part of NASA's development of a controlled ecological life support system (CELSS) for extended travel in space. Primary production and decomposition are incorporated in the model as two separate foodwebs which are coupled by carbon, nitrogen, and oxygen cycles. The resultant system of feedback loops creates and endogenous control system, stabilizes the model, and replicates features of a homeostatic ecosystem.

The Fourier Amplitude Sensitivity Test (FAST) is presented as an extremely efficient and practical alternative to Monte Carlo approaches for global sensitivity analysis and is used to analyze the effects of parametric uncertainty on the response of the model. The manner and degree of stress required to disrupt the endogenous control and destablize the model is qualitatively discussed. Confidence in the simulation results, given the associated parametric uncertainty, is quantified using global uncertainty analysis.

An essential consideration in the development and use of a model is the effect of uncertainties, which are inherent in any mathematical characterization of a complex system, on its performance. Two factors are important in such an assessment: the level of uncertainty in each parameter and the sensitivity of the model prediction to the parameter. For example, the value of a parameter may be uncertain to a large degree but have little influence on the performance of the model, or the situation may be reversed. Furthermore, the effects of several parameters varying simultaneously may have a much greater influence combined than individually. A sensitivity analysis which accounts for all feasible combinations of parameters is specified as global.

For design purposes the effects of uncertainty on the output of a model, including the extremes, must be known. All feasible combinations of parameter values can be represented by points that define a (parameter) vector space. These points map out

a space of corresponding output vectors. In order for the design process to be successful, this mapping must be reasonably well understood; unfortunately, the relationship between the two vector spaces is usually extremely complex and rarely one to one [Young 1982]. Since complex simulations such as the ecosystem model must be solved numerically, the response surface must be characterized by a finite set of parameter combinations. The size of this set of points will be limited further by the increase in model complexity and computation cost per solutions as the development of a CELSS progresses.

The Monte Carlo method describes a random process in an explicit manner that provides extreme flexibility and robustness. The technique can characterize essentially any stochastic process by calculating the system's response to randomly chosen combinations of parameter values until the distribution of the output exhibits sufficient uniformity to be analyzed statistically. Although the method is inherently inefficient, it is acceptable because of its ability to use a binary performance criterion to determine the relative importance of variations in specific parameters on the system's behavior [Auslander et al., 1982].

The same information can be obtained much more efficiently using a global sensitivity/uncertainty analysis developed and refined by Cukier, Shuler and co-workers [Cukier et al., 1973, 1975, 1978]. The method was further improved and incorporated in a general purpose FORTRAN program by Koda, McRae, and co-workers [Koda et al. 1979; McRae et al., 1982]. The methodology of the FAST program is discussed in a general manner and is demonstrated using the ecosystem as an example. The Fourier Amplitude Sensitivity Analysis (FAST) provides an almost automatic global sensitivity/uncertainty analysis through the implementation of a general purpose program that:

- readily accommodates arbitrarily large variation in up to 50 parameters.

- provides greater statistical accuracy than the Monte Carlo method given the same number of trial solutions.

- calculates the partial variance for each parameter: a normalized measure of each parameter's relative contribution to the total variance.

- provides a means to determine which parameters are not independent with reasonable ease and an economical amount of computer time.

FAST generates a pattern in the form of a search curve and from this selects a sequence of unique points that cover parameter space. Moreover, FAST analyzes the sequential and ensemble characteristics of the output values that are generated from the parameter vectors. Because of this additional source of information and because FAST samples unique points, it can provide a more complete and efficient analysis than Monte Carlo based methods.

The search curve is a one-dimensional manifold generated by two orthogonal, periodic functions of a new parameter, s, and a unique frequency, w(i), that is associated with one of the random parameters. As s varies, the search curve simultaneously carries

the parameters through their full range of uncertainty and thus travels throughout parameter space. Since this curve is used to vary the parameters as a single function of s, the model's response can be analyzed as a stochastic process or time sequence rather than merely an ensemble of points. The practical advantages of this are two-fold: first, the integral over the domain of uncertainty can be represented as a line integral, and second, the sequence of output values becomes periodic and the relative influence of each parameter on the model's performance can be assessed by analyzing the power spectrum of the output.

As the name implies, the applications of this approach have used sine functions of w(i) and s to vary the random parameters and finite Fourier analysis to decompose the output values. Cukier and co-workers have shown the search curve to explore parameter space thoroughly and systematically [Cukier et al. 1975]. The density of the output distribution depends on the set of frequencies with which the parameters are carried across the range of uncertainty. The frequencies determine the overall length of the curve and the necessary number of trial solutions.

Auslander, D.M., Spear, R.C., and Young, G.E. 1982. "Application of control theory to dynamic systems simulation." NASA-CR-166383. NASA-Ames Research Center, Moffett Field, California.

Cukier, R.I., Fortuin, C.M., Shuler, K.E., Petschek, A.G., and Schaibly, J.H. and 1975. "Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I. Theory." J. Chem. Phys.
59:3873-3877.

Cukier, R.I., Schaibly, J.H., and Shuler, K.E. 1975. "Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. III. Analysis of the approximations." J. Chem. Phys. 63:1140-1149.

Cukier, R.I., Levine, H.B., and Shuler, K.E. 1978. "Nonlinear sensitivity of multiparameter model systems." J. Comp. Phys. 6:1-42.

Koda, M., McRae, G.J., and Seinfeld, J.H. 1979. "Automatic sensitivityanalysis of kinetic mechanisms." Int. J. of Chem. Kinetics 11:427-444.

McRae, G.J., Tilden, J.W., and Seinfeild, J.H. 1982. "Global sensitivity analysis - A computational implementation of the Fourier Amplitude Sensitivity Test (FAST)." Computers and Chem. Eng. 6:15-25.

THE PARAMETRIC SENSITIVITY OF THE SEA-TO-AIR FLUX OF DIMETHYLSULPHIDE IN THE SOUTHERN OCEAN.

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Dimethylsulphide (DMS) is an important sulphur-containing atmospheric trace gas of marine biogenic origin. It is present in oceanic surface waters at concentrations sufficient to sustain a considerable net flux to the atmosphere which is currently estimated to be 0.5±0.3 Tmol Syr compared to the global natural (marine + terrestrial + volcanic) flux estimate of sulphur to the atmosphere of 0.78 Tmol Syr^{-1}.

Charlson et al. [1987] have suggested that a major source of sulphate aerosol and cloud condensation nuclei (CCN) over the oceans is the DMS produced by planktonic algae in seawater. Because the formation of clouds is sensitive to CCN density, it has been postulated that biological regulation of the climate is possible by affecting albedo and thus the Earth's radiation budget. This would be due to the effect of temperature and solar radiation on phytoplankton growth; however, it is still unclear whether the change in albedo will cause a positive or negative feedback on climate.

The Southern Ocean is relatively unpolluted and thus the production of sulfate aerosols will be mainly due to the biogenic source of DMS. Measurements made at Cape Grim, Tasmania (40° 41'S, 144°41'E) by Ayers et al. over a twenty month period have confirmed the connection between atmospheric DMS and aerosol sulphur species - a significant part of Charlson et al. hypothesis.

In order to analyse the dynamics of DMS production in the mixed layer of the Southern Ocean, we have adapted a compartment model of the planktonic food web and included the production, bacterial consumption, chemical transformation, and ventilation of DMS to the atmosphere (Gabric *et al.* 1993). The model consists of eight state variables, three of which are abiotic: dissolved inorganic N, DMS, and DMSP (the precursor compound to DMS). All state variables are averaged over the mixed layer depth. The biotic compartments comprise the primary producers (generic phytoplankton) and four consumer groups (bacteria, zooflagellates, nonphotosynthetic protozoan and micro and mesozooplankton). The flow of nitrogen and sulphur between the various compartments is described by a system of eight coupled ordinary differential equations

Despite the fact that the ecological structure of the model has been kept as simple as possible, these equations contain over thirty biological and physical parameters. Since the reliability of predictions of multiparameter ecological models, such as the system presented here, can be properly gauged only given a knowledge of the sensitivity of the results to changes in rate parameters, a sensitivity analysis has been conducted on the most important parameters of the model. In particular, attention has been placed on those parameters that may be affected by climate perturbation, for example, changing sea temperature and wind speed.

In a first approach, in order to understand which parameters should be known to great accuracy and which can permit some degree of uncertainty, we have systematically varied each of the biological model parameters by plus or minus 50% from the "reference" value. The metric we have used to gauge sensitivity is the absolute difference in the time integrated DMS concentration calculated with upper and lower estimates of each parameter.

The result of this empirical analysis is that the time-integrated DMS prediction is most sensitive to the parameters k23: the maximum phytoplankton N uptake rate, k3: involved in the link between phytoplankton and protozoa, γ: the algal S:N ratio, and the initial mixed layer nitrogen concentration.

The k23 and the γ parameters are both strongly correlated with the climate change. The maximum phytoplankton N uptake rate is a function of sea-temperature; the algal S:N ratio can be altered because large-scale shifts in phytoplankton community composition can occur, due to changes in primary productivity as temperature, CO_2 and nitrogen flux from the atmosphere increase. Increased biomass and large relative changes in population of algae due to differential nutrient uptake by different species have already been noted in the North Sea.

In a second stage we have conducted a more elaborate analysis, following the method of Morris, of these parameters as they affect the sea-to-air flux of DMS, computed as the product of the sea-to-air exchange coefficient and DMS sea-water concentration.

Together with the biological parameters k3, k23, γ, the initial mixed layer nitrogen concentration (DIN) has also been examined. While not a parameter, but rather an initial condition, DIN has been included as it will likely be affected by climate perturbation. The influence of sea surface temperature, which affects both the phytoplankton growth rate and the exchange coefficient of DMS, has also been examined.

The guiding philosophy in the computational experiment presented by Morris, is that a major role of a preliminary computational experiment is to determine, within reasonable uncertainty, which input parameters may be considered to have effects which are (a) negligible, (b) linear and additive, and (d) nonlinear or involved in interactions with other inputs.

The method is based on an experimental plan, composed of individually randomised one-factor-at-a-time designs, with the purpose of collecting random samples from the distribution of "elementary effects" associated with each input parameter.

The elementary effect of the *ith* input is defined as the difference between two evaluations of the output y, one at selected values of input x_i , and the other after increasing x_i by a predetermined quantity Δ. The finite distribution of elementary effects associated with the ith input parameter will be denoted F_i.

A large (absolute) measure of central tendency for F_i indicates an input parameter with an important "overall" influence on the output. A large measure of spread indicates an input whose influence is highly dependent on the values of the other inputs-i.e., one involved in interactions or whose effect is nonlinear. In particular, estimates of the means and standard deviations of these distributions will be used as indicators of which inputs should be considered important.

Several different designs can be constructed to provide random samples from each of these distributions on which such estimates may be based. In simplest form, since an elementary effect involves the evaluation of y twice, the total computational effort to obtain a random sample of r values from each F_i is $n = 2rk$ runs. Thus, because the "economy" of a design is defined to be the number of elementary effects it produces divided by the number of experimental runs, this sampling scheme has an economy of 1/2. However more economical designs can be constructed if some runs are used in computing more than one elementary effect. Following an idea proposed by Morris, we have constructed an experiment with economy $kr/r\,(k+1)$.

Once we have collected elementary effects for each input, mean and variance of F_i have been estimated using the same estimator as would be used with an independent random sample.

Results of the experiment have been analysed by plotting estimated mean and standard deviation for each input. None of parameters studied has both mean and standard deviation close to zero, that is the DMS flux prediction is indeed sensitive to these parameters, confirming the preliminary analysis.

Input parameters γ and temperature have mean elementary effects that are substantially different from zero while having small standard deviations, that is both have a large *direct* effect on the flux prediction. This is reasonable as γ defines the cell DMSP concentration and temperature impacts both the exchange coefficient and the rate of growth of phytoplankton. The parameter k23 (phytoplankton nutrient uptake rate) has both mean and standard deviation significantly different from zero, which implies that k23 has both a direct and indirect effect on the model output. Again this is understandable as nutrient uptake rate will not only affect the magnitude of DMS produced, but also influence the timing of the peak in DMS through interactions with the other trophic species in the food web. Initial nitrogen and k3 parameters have mean values very close to zero but large values of variance, indicating potentially extensive patterns of interaction with other parameters.

REFERENCES

Charlson RJ, Lovelock JE, Andreae MO and Warren SG (1987) Oceanic phytoplankton, atmospheric sulphur, cloud albedo and climate. Nature, 326, 655-661.

Gabric AJ, Murray N, Stone L and Kohl M (1993) Modelling the production of dimethylsulphide during a phytoplankton bloom. J. Geophys. Res. 98, C12, 22805-22816.

FIRST ORDER SENSITIVITY ANALYSIS OF A DISTRIBUTED PARAMETERS ECOLOGICAL MODEL.

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Methods

Sensitivity and uncertainty analysis have become standard tools in water quality modelling (1), but they have been mainly applied to lumped parameters models, which do not enable one to describe the evolution of a complex system as a coastal basin, where the geomorphology and the transport processes lead to a spatial differentiation. A more realistic description of these systems can be reached by combining the transport processes and the chemical and biochemical reactions in the mass-balance equations, and solving the system of partial differential equations so obtained.

This paper presents a first-order sensitivity analysis of a reaction diffusion model, based on the linearization around the standard trajectory of the system, written in vector form:

$$\frac{\partial \bar{c}}{\partial t} = \frac{\partial (K(x)\bar{c}/\partial x)}{\partial x} + \bar{f} \qquad (1)$$

where $K(x)$ is a space varying diffusivity, $\bar{c}$ is the state vector and $\bar{f}$ is a non linear vector function which expresses the local rate of change due to sources and sinks and to the chemical and biochemical transformations.

After discretization of the spatial dominion in n_x cells, the dimensions of the state space of the dynamic system become n_x x n_v and those of the parameter vector become n_x x n_p, where n_v are the number of state variables and n_p the number of parameter in each cell. Therefore, the dimensions of the augmented state vector become nx x (nv + np) and one should solve n_x^2 x n_p vector differential equations (2) in order to estimate the effects of each single variation of any parameter in any cell of the spatial dominion:

$$\frac{d\bar{S}_{ix,jx,ip}}{dt} = \frac{\partial f_{ix}}{\partial \bar{c}_{ix}} \bar{S}_{ix,jx,ip} + \frac{\partial f_{ix}}{\partial p_{jx,ip}} + D_{ix-1}(\bar{S}_{ix-1,jx,ip} - \bar{S}_{ix,jx,ip}) + D_{ix}(\bar{S}_{ix,jx,ip} - \bar{S}_{ix,jx,ip}) \qquad (2)$$

In eq. (2) $\bar{S}_{ix,jx,ip}$ represents the sensitivity of the state variables in the grid point *ix*, in respect of the parameter *ip* in the grid point *jx*. D_{ix}, expressed in [t^{-1}], is a dispersion coefficient which embodies the spatial step. Nevertheless, in most ecological applications, the same local rate of change $\bar{f}_{ix}$ and the same vector of parameters $\bar{p}_{ix}$ are used throughout the spatial dominion and one is usually concerned with estimating the effects of the simultaneous variation around its nominal value of one component $p_{ix,ip}$ of $\bar{p}_{ix}$ in every cell. In this case, the overall effect can be estimated by summing up the single ones. After collecting the local Jacobian matrix and noting the explicit partial derivatives vanish for jx≠ix, one obtains:

$$\frac{d\bar{S}_{ix,ip}}{dt} = \frac{\partial f_{ix}}{\partial \bar{c}_{ix}} \bar{S}_{ix,ip} + \frac{\partial f_{ix}}{\partial p_{ix,ip}} + D_{ix-1}(\bar{S}_{ix-1,ip} - \bar{S}_{ix,ip}) + D_{ix}(\bar{S}_{ix,ip} - \bar{S}_{ix,ip}) \qquad (3)$$

where $\bar{S}_{ix,ip} = \sum_{jx=1}^{nx} \bar{S}_{ix,jx,ip}$ is the overall sensitivity.

Once the sensitivity equations have been analytically derived for the lumped parameter model, the solution of eq. 3 is straightforward and computationally convenient, because each overall sensitivity can be treated as a supplementary state vector in the transport subprogram.

The method has been applied to a 1-D, depth averaged, finite difference model which follows seven state variables (phytoplancton and zooplancton density, ammonia, nitrate and reactive phosphorous concentration, organic detritus and dissolved oxygen) forced by a continuous nutrient load and a light-temperature temporal pattern which reproduces the average meteoclimatic conditions of one of the main channels of the lagoon of Venice, which connects the Industrial zone with the mouth of Malamocco. The channel is included in a monitoring network, where monthly samplings of Tempeature, Ammonia, Nitrate, Total Phosphorous, Chla have been carried on since 1986, providing a consistent time series of water quality data (2). It is well mixed by the tidal agitation, which is accounted for by a vector of turbulent diffusivities. The model has been developed during a long term multidisciplinary research, aimed at defining a 3D combined transport-water quality model of the central part of the lagoon of Venice (3), (4).

Results and discussion

The method has been tested by comparing the deviations from the yearly standard trajectory computed by using the sensitivities and the one obtained by actually increasing each parameter of 2% of its nominal value. As an example, Fig. 1 shows the deviations from the standard phytoplankton due to a variation of its maximum growth rate, in the cell where the nutrient source is placed, Station n. 7 in the network As one con see, the estimated state and the actual one match very well for most of the year. The slight disagreement in the spring is due to the non-linear predator-prey interaction.

Sensitivities has then been used for ranking the parameter, according with their first-order effect on the output variables, Phytoplankton, Ammonia, Nitrate, and Reactive Phosphorous, denoted with *ivo*, in the cells corresponding to the sampling sites. The following dimensionless index has been taken as a measure of the global effect on model output:

$$\delta_{ix,ip} = \sqrt{\sum_{ivo=1}^{nvo} \sum_{it=1}^{nt} \left(\frac{\left(S^2_{ivo,ix,ip}(it) \Delta^2_{ip} \right) / nt}{\bar{c}^2_{ivo}} \right)} \qquad (4)$$

The index represents the mean deviation, in the time interval T = Δt *nt*, from the standard trajectory due to a change Δ_{ip} of the component *ip* of the vector of parameter, in a space spanned by the variables divided by their mean values. Results, shown in Fig. 2 for the three cells corresponding to the sampling sites numbered as 7, 8, 9 in the network, partially confirmed the previous analysis on the lumped parameter model, and put in evidence the role of the higher trophyc level in controlling the dynamic of the system in eutrophyc conditions. The two highest deviations are due to the zooplancton grazing and mortality, while the two half-saturation constants, Kn and Kp, are of little importance. The most sensitive cell, is the source cell, while the less sensitive is St. 9, the closest to the sea.

References
(1) Beck, M.B. 1987. Water quality modelling: a review of the analysis of uncertainty. Water Resources Research, Vol. 23, N. 8, 1393-1442
(2) Fant M., 1995. Analisi statistica di serie storiche chimiche ed ecologiche nelle acque lagunari. Master Thesis in Environmental Sciences, Univ. of Venice.
(3) Dejak, C., Mazzei, L.I., Meregalli, L., Pecenik, G. 1987. Development of a mathematical eutrophycation model of the lagoon of Venice. Ecol. Modelling, 37, 1-20.
(4) Pastres, R., Franco Davide, Pecnik G., Solidoro C., Dejak, C. 1995. Using parallel computer in environmental modelling: a working example. Ecol. Modelling, 80, 69-85.

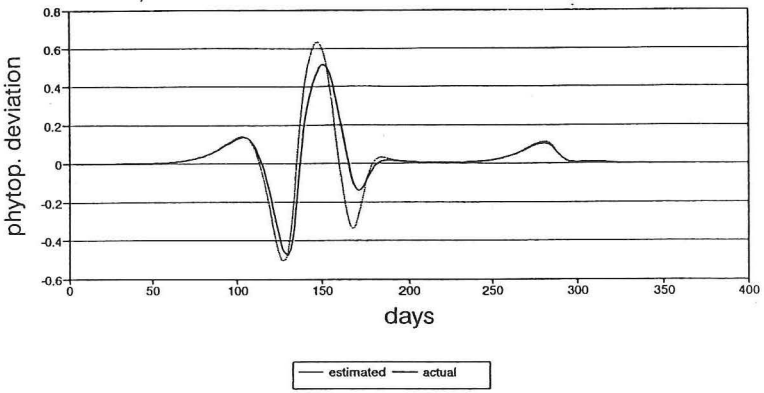

Fig. 1. Deviation from the standard phytoplankton run, in the source cell, due to a 2% increase of its maximum growth rate. Comparison between estimation based on sensitivities and actual differences.

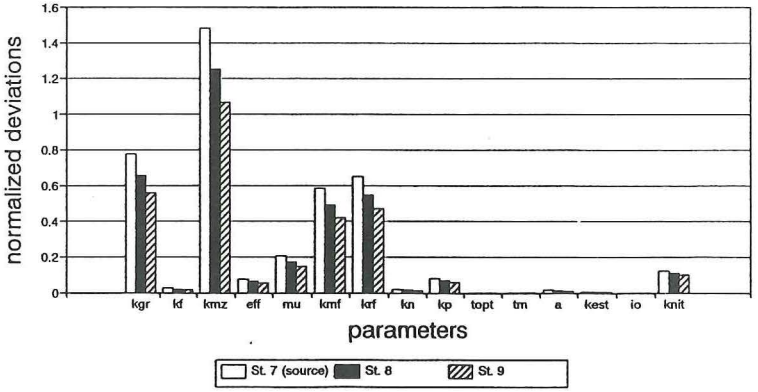

Fig. 2. Mean dimensionless deviation from model output due to a 2% increase of each parameter in three cells. St. 7 is the source cell, St. 8 and St. 9 are placed downward. The first four parameters from left are directely linked with Zooplankton dynamic, the following to the Phytoplancton one.

PROBABILISTIC SENSITIVITY MEASURES AS APPLIED TO SATURATED AND UNSATURATED FLOW AND TRANSPORT

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INTRODUCTION

First- and second-order reliability algorithms (FORM and SORM) have been used for probabilistic analysis of subsurface flow and transport in porous media over the last decade or so. The reliability algorithm is coupled with an existing analytical or numerical solution to provide an estimate of probability (for example, an estimate of the probability that some target contaminant concentration is exceeded at some point and time). Perhaps more importantly, the reliability algorithm provides sensitivity measures which identify the most important uncertain variables in the analysis and which incorporate the probabilistic nature of FORM and SORM (thus they are more comprehensive than typical deterministic sensitivity measures).

Research by the authors and others over the last few years has been focused sequentially on applying FORM and SORM to the following problems and model solutions: relatively simple analytical solutions of flow and transport (1), numerical models of groundwater flow in the saturated zone (2), analytical and numerical solutions of one- and two-dimensional transport in the saturated zone (3) and (4), one-dimensional flow and transport in the unsaturated zone (5), and two-dimensional flow and transport in the unsaturated zone (6). The sensitivity information is often the main focus in these works and identifies the most important uncertain variables for a wide range of problem geometries, boundary conditions, and statistical assumptions. The influence of spatial correlation for one variable, or the influence of cross correlation between variables may also be studied. Natural geologic deposits are highly variable, heterogeneous, and difficult to characterize. Thus, material properties are very uncertain. Typical variables that must be characterized for subsurface flow and transport problems include the hydraulic conductivity (or permeability) (K), the porosity (n), the dispersion coefficient (D), and reaction terms such as distribution coefficient, and bulk density. Little information exists concerning the statistical characteristics of most of these variables; therefore, in order to study these variables and their influence on the probabilistic outcome, a wide range of statistical assumptions are made for each variable.

BACKGROUND OF FORM AND SORM

FORM and SORM have been used in structural analysis problems for years. Papers referenced above provide a full treatment of the theory as applied to subsurface flow. The technique requires defining a performance function such that "failure" occurs when the function is less than zero. An estimate of the probability that "failure" occurs is sought. For example, the

performance function for a transport model might be: $g(X) = C - C(x,y,t)$. C is a target concentration, and $C(x,y,t)$ is the concentration evaluated by the model at location (x,y) and time t (utilizing the vector of uncertain variables X). If $C(x,y,t)$ is greater than C, "failure" occurs. Thus, the FORM or SORM algorithm estimates the probability that $C(x,y,t)$ is greater than or equal to C.

The solution is obtained by defining second-moment statistics for all uncertain variables in the model, transforming the performance function into uncorrelated standard normal space, and finding the point y* on the surface $g(X)=0$ that is closest to the origin in standard space. This point y* defines the "most likely failure point", and the distance between the origin and y* is known as the reliability index (beta). A first-order (FORM) or second-order (SORM) estimate of the probability defined by the surface $g(X)=0$ is made at y*. A constrained optimization algorithm is used to determine the value of y*, and partial derivatives of the function g(X) with respect to each uncertain variable are calculated. These partial derivatives are used in a formulation involving the Jacobian of the transformation to standard space in order to provide probabilistic sensitivity information (e.g., Jang, et al, 1994). These sensitivity measures indicate, for example, the sensitivity of the probabilistic outcome to equally likely changes in any of the uncertain variables.

FORM and SORM are computationally efficient compared to Monte Carlo simulation for many scenarios. They are particularly attractive for low probability events and because they directly provide sensitivity information. However, FORM and SORM only provide an estimate of the probability for a single event of interest, whereas Monte Carlo simulation can simultaneously provide probability distributions at many locations. FORM tends to overestimate the probability in some cases (4), but the sensitivity information is not affected (the sensitivity measures are only a function of y* and the partial derivatives).

APPLICATIONS AND RESULTS

In the interest of brevity, only major conclusions from numerical modeling studies of flow and transport are discussed here. Two types of flow and transport situations have been investigated: saturated and unsaturated.

In the saturated zone, the typical numerical model is a two- or three-dimensional finite difference or finite element model. Each element or node may have uncertain material and hydraulic properties associated with it. Spatial correlation between, for example, element hydraulic conductivities may also be defined. A finite element solution (3) was used to investigate the importance of uncertain hydraulic conductivity and transport parameters, and their spatial correlation. The FORM results indicated that the distribution coefficient and bulk density were most important to the probabilistic outcome in many transport situations; however, longitudinal dispersivity can be very important if it is defined as a single, global uncertain variable and not a spatially variable parameter. Significantly, the spatial correlation range for hydraulic conductivity did not have significant impact on the probabilistic outcome for the examples studied. It should be noted that calculating the partial derivative terms (used in the optimization algorithm and for evaluating sensitivity measures) can be computationally intensive when a

numerical solution model with hundreds of uncertain variables is considered (e.g., each element has uncertain hydraulic conductivity).

In the unsaturated zone, the numerical solution for subsurface flow is non-linear and the porous media properties are related in complex ways which are only imperfectly modeled by current theories. Recent works (5) and (6) have utilized FORM to study the importance of the van Genuchten hydraulic model parameters and other flow and transport variables. Results indicate that, in general, the probabilistic outcome is very sensitive to likely changes in the saturated water content; the diffusion coefficient, residual water content, and first-order decay coefficients do not seem to be significant uncertain variables for transport in the unsaturated zone. For probabilistic modeling of the unsaturated zone, difficulties arise in defining the exact nature of the uncertain variables, and in utilizing FORM with non-linear numerical schemes. When the uncertainty of the variables is high, the optimization scheme used in FORM may not converge when used in conjunction with the non-linear numerical solutions.

CONCLUSIONS

FORM and SORM offer some advantages for probabilistic sensitivity analysis of subsurface flow and transport. Although the techniques utilize approximations for estimating probability, the sensitivity information is not influenced by the approximation and can be used to indicate the most important uncertain variables in a problem. This sensitivity information can be very useful for guiding field and laboratory sampling programs, so that effort can be concentrated on reducing the uncertainty of those variables that are most important to the probabilistic outcome.

REFERENCES

(1) Sitar, N, J. Cawlfield, and A. Der Kiureghian, First-order reliability approach to stochastic analysis of subsurface flow and contaminant transport, Water Resour. Res., 23(5), 1987.

(2) Cawlfield, J., and N. Sitar, Stochastic finite element analysis of groundwater flow using the first-order reliability method, in Consequences of Spatial Variability in Aquifer Properties, IAHS, 1988.

(3) Cawlfield, J. and M-C. Wu, Probabilistic analysis for one-dimensional reactive transport in porous media, Water Resour. Res., 29(3), 1993.

(4) Jang, Y-S, N. Sitar, and A. Der Kiureghian, Reliability analysis of contaminant transport in saturated porous media, Water Resour. Res., 30(8), 1994.

(5) Cawlfield, J., and J. Piggott, Probabilistic sensitivity analysis of one-dimensional unsaturated non-hysteretic flow in loamy sand, Proceedings, 14th Annual AGU Hydrology Days, 1994.

(6) Cawlfield, J., and S. Boateng, Stochastic 2-D simulations and sensitivity analysis of variably saturated flow and transport using reliability methods, AGU Spring Meeting, 1995.

UNCERTAINTIES IN MODELLING WATER FLOWS THROUGH FRACTURED ROCK

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Background and Objectives

Groundwater modelling is widely recognised as a potentially powerful tool for aiding site investigations, undertaking risk assessment and identifying possible remediation options associated with contaminated land. Industry, regulators and academics worldwide have developed and used a variety of groundwater models for various different purposes and a number of good models exist and are often publicly available.

It is also recognised, however, that groundwater models may vastly oversimplify sub-surface flow and transport phenomenon, either because insufficient data are available to adequately characterise the hydrogeology, or because the processes describing these phenomenon are poorly understood.

Consequently, most groundwater studies tend to assume that the soil or rock matrix is a continuous medium, often even if the geology is known to be heterogeneous or fractured, because the available data are inadequate to allow more sophisticated models to be used.

A few more advanced models describing flow and transport in fractured media have been developed and concepts such as 'dual-porosity' and the problems associated with parameter scaling from small to large scale processes are active areas of current research.

Few fractured rock models have been properly evaluated, owing to lack of suitable data. However, it is possible to examine the potential usefulness of a model by undertaking an uncertainty and sensitivity analysis.

The objective of the current study is to assess whether the complexity of a fractured rock model is justified for a specific aquifer system, given the available data, and whether the uncertainty in the data causes variations in the predictions which are too large for the model to be useful.

Model Area

The current study focuses on a fractured Triassic sandstone aquifer in the Northwest of England, known as the Sherwood sandstone, which is a major water supply aquifer for the region. A model has been set up for this aquifer, and extends over an area of 15x16 km, including the estuary of the Mersey. Data for the area have been obtained from published information although several gaps in the data exist. In particular, characterisation of the fracture pattern is a difficult problem which leaves a considerable uncertainty in the frequency, orientation and size of the fractures.

The sandstone is between approximately 100 to 200m deep and is overlain by layers of clay and surface alluvium which comprise up to the top 30m of the surface geology. In some places either the clay and/or alluvium are absent and occasionally the sandstone outcrops at the land surface.

Model Data

Methods are available for characterising fractures, including some fairly advanced technology such as seismic profiling. However, many of these methods are expensive and tend to be used more widely in the oil and nuclear industries, where much deeper aquifers are considered and the objectives are to characterise oil reservoirs and safe nuclear waste repositories. The problems associated with contaminated land tend to be confined to near surface geologies such as the Sherwood sandstone.

The data used for this study are extremely sparse. They are obtained from stereogram projections from three quarries in the model area which give broad information about the likely distribution, orientation and apertures of the fractures that are exposed on the quarry faces. These, together with some literature data from the area, have been used to estimate the fracture pattern over the whole model area.

Methods

The model used for this study is TRAFRAP-WT. This is a two dimensional model for fluid flow and solute transport in fractured rock from the International Groundwater Modelling Centre, Colorado, USA and has been set up for the aquifer. It has been run to give water table heights, water flows and travel times under various conditions.

The sensitivity of the model to the fracture data is assessed using a statistical experimental design to plan the model runs required to cover the uncertainty in the input fracture data and other parameters. Statistical analyses are then applied to the model results to determine which parameters are most important in terms of influencing the overall model predictions, thus providing an assessment of the overall uncertainty.

The uncertainty in the available data is then used to assess whether it is worth obtaining further data, or whether the error bands are too large to make this cost-effective.

Predictions of water table heights and travel times from this model are also compared against results from a standard 'continuous medium' model of the same area, in order to assess whether the complexity of a fractured rock model is justified for this aquifer system.

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A Variational Method for Determining Uncertain Parameters and Geometry in Hydrogeology

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Introduction

The stationary groundwater flow in geological media is obtain by determining the hydraulic potential $\phi(\bar{r})$, solution of the 3-D elliptic equation (see [1])

$$div\,(K(\bar{r})\ grad\,\phi(\bar{r})) = Q(\bar{r}) \tag{1}$$

where $K(\bar{r})$ is the hydraulic conductivity and $Q(\bar{r})$ the source term. The potential $\phi(\bar{r})$ is submitted to three main causes of uncertainty : the highly variable value of $K(\bar{r})$, the values of boundary conditions and the geometry of the layers of the medium. However, some measures $\phi^m(\bar{r}_\alpha)$ at locations $\bar{r}_\alpha$ are known by field experiments. The goal is to determine the parameters providing a computed solution $\phi^c(\bar{r})$ fitting at best the measured values. We use for this inverse problem the Gauss-Newton method which needs the knowledge of the sensitivity matrix [2]; [3].

Sensitivity coefficients

We have developed a first order variational method to determine analytically the variation of the potential $\delta\phi(\bar{r}_\alpha)$ at $\bar{r}_\alpha$ due to variations of the following parameters : $\delta Q(\bar{r})$ (sources), $\delta Y(\bar{r})$ ($Y(\bar{r}) = ln\,K(\bar{r})$: log conductivity), $\delta f(\bar{r})$ (values of the boundary conditions : Dirichlet or Neumann) and $\delta\bar{a}(\bar{r})$ (position of the interfaces between geological layers).
This method is based on the knowledge of the solution $\phi_i^*(\bar{r}\,|\,\bar{r}_\alpha)$ of the adjoint problem in a particular geological layer. For the i^{th} layer, we have

$$div\,(K_i(\bar{r})\ grad\,\phi_i^*(\bar{r}\,|\,\bar{r}_\alpha)) = \delta(\bar{r} - \bar{r}_\alpha) \tag{2}$$

The boundary conditions of this latter problem may be chosen such as the expression of $\delta\phi(\bar{r}_\alpha)$ depends only on the variations of the parameters $\delta Q, \delta Y, \delta f$ and δa and not on $\delta\phi$ itself and $\delta\phi^*$. We showed moreover that the choice of these boundary conditions determines

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the portion of interfaces, between the geological layers, allowed to move in order to fit the measured data.
A general analytical expression of $\delta\phi(\bar{r}_\alpha)$ has been obtained by a variational formulation. By considering the following hypotheses : point sources, quasi-planar surfaces, constant displacements of surfaces parallel to their normal ($\bar{n}$) and values of hydraulic conductivity and boundary conditions constant in each geological layer, the variational formula becomes for the i^{th} layer

$$\begin{aligned}\delta\phi(\bar{r}_\alpha) &= \sum_{\bar{r}_k \in \mathcal{V}_i} \delta q_k \, \phi_i^*(\bar{r}_k \,|\, \bar{r}_\alpha) + \int_{S_i^N} \phi_i^*(\bar{r} \,|\, \bar{r}_\alpha) \, dS \; \delta f_i \\ &+ \left[K_i \int_{S_i^N} \phi_i^*(\bar{r} \,|\, \bar{r}_\alpha) \; \phi_n(\bar{r}) \, dS \; - \sum_{\bar{r}_k \in \mathcal{V}_i} q_k \, \phi_i^*(\bar{r}_k \,|\, \bar{r}_\alpha) \right] \delta Y_i \qquad (3) \\ &+ K_i \int_{S_i^N} \left[\bar{\nabla}\phi \bar{\nabla}\phi_i^*(\bar{r} \,|\, \bar{r}_\alpha) - \phi_i^*(\bar{r} \,|\, \bar{r}_\alpha)(\bar{n}.\bar{\nabla})\phi_n(\bar{r}) \right] dS \; \delta a_i\end{aligned}$$

where $\mathcal{V}_i$ is the domain of the i^{th} layer; S_i^N is the portion of surface limiting $\mathcal{V}_i$ and where a Neumann boundary condition is imposed; $\phi_i^*(\bar{r} \,|\, \bar{r}_\alpha)$ is the adjoint solution of Eqn (2) in $\mathcal{V}_i$; $\phi_n(\bar{r})$ is the normal derivative of $\phi(\bar{r})$ and $Q(\bar{r}) = \sum_k q_k \delta(\bar{r} - \bar{r}_k)$. This result may be written as

$$\delta\phi(\bar{r}_\alpha) = \sum_{j=1}^{N_p} H_{\alpha j} \; \delta p_j \qquad (4)$$

where $H_{\alpha j}$ is an element of the sensitivity matrix H and δp_j a component of the N_p-dimensional vector $\delta\bar{p}$ of variation of the parameters. The originality of our sensitivity analysis, in comparison with other sensitivity analyses found in the literature ([2] and [3]), is to take into account the effects of a variation of the surface position (δa_i) as shown in Eqn (3). These effects are added to the effects of a variation of source intensities (δq_k), hydraulic conductivity (δY_i) and boundary conditions (δf_i).

Inverse problem - iterative search

We consider a function F which is the product of two probability density functions. The first one (F_m) represents the conditional probability of finding the computed solution $\phi^c(\bar{r}_\alpha) + \delta\phi^c(\bar{r}_\alpha)$, given a certain vector $\delta\bar{p}$ of variation of the parameters, in the error interval of the measure $\phi^m(\bar{r}_\alpha)$ at location $\bar{r}_\alpha$. The second one (F_p) is the probability of having each parameter p_j in the neighbourhood of its best estimate $p_j^{best\ estim.}$.

$$F = F_m \; F_p = Pr(\phi^c + \delta\phi^c \mid \delta\bar{p}) \; Pr(\delta\bar{p}) \qquad (5)$$

We have considered, as an example, independent gaussian probability density functions of means $\phi^m(\bar{r}_\alpha)$ with standard deviations σ_α (error of measure) for F_m; and means $p_j^{best\ estim.}$ with standard deviations $\sum_j$ for F_p. Introducing (4) in (5), we obtain an expression of F depending only on $\delta\bar{p}$. This last expression is maximised and provide a linear algebraic system of equations with unknowns δp_j. This system is solved by using direct methods and gives the solution of the inverse problem. However, the expression (4) of $\delta\phi^c(\bar{r}_\alpha)$ is valid only for a small variation $\delta\bar{p}$. This restriction may induce errors in the values of $\delta\phi^c(\bar{r}_\alpha)$. Therefore,

having computed the solution of the inverse problem, we modify the values of the parameters and determine new solutions of $\phi^c(\bar{r})$ and $\phi_i^*(\bar{r} \mid \bar{r}_\alpha)$. With these new solutions, we calculate from Eqn (3) new values of $\delta\phi^c(\bar{r}_\alpha)$ and so on. We consider a small number of iterations of the whole process in order to approach the maximum of F where Eqn (4) is accurate.

Numerical results

The preceding technique has been applied to a simple test problem in a parallelepipedic domain with three horizontal layers of different conductivity and with a point source. A Dirichlet condition is imposed on the upper surface and Neumann conditions on the other surfaces. We have discretised the domain with 1000 nodes. We mention here that our program handles also more general domains made of any curved interfaces by transforming these domains to parallelepipedic ones after the use of curvilinear coordinates.
A sensitivity analysis has given the following results : The sensitivity coefficient of hydraulic conductivity is generally dominant. The sensitivity coefficients of the sources and boundary conditions may be as large as those of hydraulic conductivity (even larger) if the points of measures are near the locations of the sources or near the boundaries. For an uniform flow, the sensitivity coefficients of the surface position are zero or negligible. When the flow is not uniform (for instance due to an intensive pumping at a well), these coefficients may be as large as the sensitivity coefficients of the sources and of the boundary conditions.
Next, we have considered one by one the variation of the parameters. Knowing the solution of a "modified" problem $\phi^c_{mod}(\bar{r})$ (obtained after modification of one of its parameter), we consider at some locations $\bar{r}_\alpha$ the values of $\phi^c_{mod}(\bar{r})$ as values of hypothetical measured data $\phi^m(\bar{r}_\alpha)$. We start with an initial problem, we impose these "measured" data and we observe, during the iterations, the modification of the parameter. When a modification of surface positions is concerned, the curvilinear coordinates are each time computed, taking the new geometry into account. The techniques of under- and overshooting have been in some cases applied to accelerate the convergence of the whole iterative process. Therefore, only a few iterations are needed to attain significant results.
Afterwards, we have studied the variations of all the parameters : a good behaviour of the convergence is observed when the parameters associated to the largest absolute values of the sensitivity coefficients are modified at first, the numerical simulation ending with modifications of parameters of low sensitivity.
In order to simulate realistic data, we have added a random noise on the measured data $\phi^m(\bar{r}_\alpha)$ by considering random sampling of errors from gaussian distributions with standard deviation σ_α. We have also considered larger problems with about 200,000 nodes.

References

[1] J., BEAR, *Hydraulics of Groundwater*, Mc Graw-Hill Series in Water Resources and Environmental Engineering, Mc Graw-Hill, 1979.

[2] N.-Z., SUN, W.W.-G., YEH, *Coupled Inverse Problems in Groundwater Modeling : 1. Sensitivity Analysis and Parameter Identification.*, Water Resour. Res., Vol. 26, No. 10, pp 2507-2525, 1990.

[3] N.-Z., SUN, M.-C. JENG AND W.W.-G., YEH, *A proposed geological Parametrization Method for Parameter Identification in Three-Dimensional Groundwater Modeling*, Water Resour. Res., Vol. 31, No. 1, pp 89-102, 1995.