SE0000096

Assessing scenario and parametric uncertainties in risk analysis: a model uncertainty audit

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Abstract

In the present study a process of model audit is addressed on a computational model used for predicting maximum radiological doses to humans in the field of nuclear waste disposal. Global uncertainty and sensitivity analyses are employed to assess output uncertainty and to quantify the contribution of parametric and scenario uncertainties to the model output. These tools are of fundamental importance for risk analysis and decision-making purposes.

1 Introduction

Analyses of risk and decision-making methodologies are essential elements of investigation in many human activities, ranging from engineering to socio-economics, where the planning requires suitable tools for the quantification of risk as well as for the assessment of alternative options. These analysis tools make use of computational models, simulating the system under investigation, to provide data for the analysis itself. Models are constructs meant to mimic real systems, and their intrinsic value escapes the rigor of mathematical proof. Often models approximate a natural system crudely, or there are competing models (or scenarios) of comparable plausibility for a given problem. Finally models contain input factors (parameters) affected by uncertainties. In this work we examine a process of model audit, by investigating the effect of (i) scenarios uncertainties (possible exclusive evolutions of the system under study); and (ii) parametric uncertainty (both intrinsic, such as, e.g., the time of occurrence of a geological event, or due to our poor knowledge of the system). The study focus is a risk assessment of nuclear waste disposal. A computational model predicts the maximum radiological dose for humans on the surface of the earth due to the underground migration of radionuclides from a nuclear waste disposal site. The overall predictive uncertainty about the maximum dose is partitioned into two components, between scenarios and within scenarios. Six different scenarios are considered. The model involves 54 uncertain factors (relevant physical constants of the process that are unknown, such as retention coefficients for radioactive species, length of pathways, and so on). The probability distributions of the factors and the scenarios are selected on the basis of expert judgement. The model uncertainty audit has shown that 30% of the total output variance arises from scenario uncertainty. We argue that the study, while not pretending to predict the future, helps the analyst as it shows the implausibility of catastrophic negative events that would have both high probability and high impact to change the overall picture. The FAST technique for global sensitivity analysis, which is capable of computing additive and interaction effects for all the uncertain factors of a model, has also been employed to study the impact of scenario and parametric uncertainties on the model output variability. Quantitative sensitivity indices show that, while the influence of each source of uncertainty taken singularly is small, the two sources have a strong interaction component. It can therefore be concluded that, at any time, none of the two sources of uncertainty can be fixed (as it were perfectly known) in the analysis.

2 Background

The problem of safe disposal of radioactive waste arising as a by-product of nuclear power generation is object of intensive studies since 1970s. Deep geological disposal is still the most actively investigated option, although some objections to underground storage persist today (e.g., Keeney and von Winterfeldt 1994, Shrader-Frechette 1994). It is fair to say that even after decades of research, the physico-chemical behavior of deep geological disposal systems over geological time scales (hundreds or thousands of years) is far from known with certainty.

Since 1996, with partners at *CIEMAT* in Madrid and the Physics Department at Stockholm University, we have been involved in a project for the European Commission, GESAMAC[1], whose principal aim is to make progress in capturing all relevant sources of uncertainty when predicting what would happen if deep geosphere disposal barriers were compromised in the future by processes such as *geological faulting, human intrusion,* and/or *climatic change.* We have been using sensitivity analysis (SA) and uncertainty analysis (UA) in predicting the radiologic dose for humans on the earth's surface as a function of time, how far the disposal facility is underground, and other factors likely to be strongly related to dose. This is clearly not a real, site-specific safety study, but a simplified framework in order to illustrate SA and UA methodologies.

3 The system model

The system model on which our predictions are based consists of a hypothetical underground radioactive waste disposal system represented by three coupled submodels. The first submodel assumes an initial containment time for the waste materials (only radioactive decay is considered), followed by a constant leaching rate of the radioactive inventory present at the time containment fails.

[1]GEosphere modeling, geosphere Sensitivity Analysis, Model uncertainty in geosphere modeling, Advanced Computing in stochastic geosphere simulation: see http://www.ciemat.es/sweb/gesamac/.

The third submodel — the biosphere, assumes that the radionuclides leaving the geosphere enter a stream of water from which a humans obtain drinking water, so that the dose received depends on the ratio of the drinking water consumption to the stream flow rate.

The second submodel, on which computations are mainly focused, is the geosphere. GESAMAC has released for public use a program called GTMCHEM, which uses Monte Carlo methods to simulate the transport of radionuclides by groundwater through geologic formations, represented by a one-dimensional column of porous material (consisting of one or more layers) whose properties can change along the pathway and in which different chemical reactions (homogeneous or heterogeneous) can take place. GTMCHEM incorporates a number of chemical phenomena, including equilibrium complexation in solution, homogeneous first-order chemical kinetics in solution, slow reversible adsorption, and a sink associated with filtration or biodegradation. GTMCHEM produces the peak radiologic fluxes at the end of each geosphere layer and the peak dose for each nuclide, as well as the associated time of the peak. The program may also be run with a fixed set of time points at which the fluxes and/or doses through space may be computed and stored.

GESAMAC developed a new test case called *Level E/G* (Prado et al. 1998) by creating a total of six scenarios:

- Reference (REF). It is the Level E test case, which tracks the one-dimensional migration of four radionuclides: iodine (I–129), and a chain consisting of neptunium (Np–237), uranium (U–233), and thorium (Th–229), through two geosphere layers characterized by different hydro-geological properties (PSACOIN Level E Intercomparison, NEA PSAG User's Group 1989).

- A fast pathway (FP) to the geosphere, corresponding to a geological fault passing directly through the containment chamber, or to the reduction of the geosphere pathway by erosion of the upper layer, or to the bypassing of the second layer through human activities such as digging. This scenario thus represents a substantial decrease in radionuclide travel time through a large reduction in the geosphere pathlength;

- An additional geosphere layer (AG), the opposite situation from the previous scenario. This case arises, for instance, from a retreating glacier leaving behind another barrier layer between the repository and the biosphere, or when a geological event creates an alternative pathway that is longer than that in the reference case;

- Glacial advance (GA), related to the AG scenario but arising from an advancing rather than retreating glacier;

- Human disposal errors (HDE), corresponding to deficiencies in the construction of the repository and/or in waste disposal operations leading to premature failing of the near-field barriers; and

- Environmentally induced changes (EIC), arising from human activities or geological events that indirectly are responsible for the modification of the disposal system conditions, such as the drilling of a pumping well or mining tunnel at a dangerously small distance from the containment chamber.

This test case was arrived at by creating a total of nine micro-scenarios—three in each of the categories *geological changes, climatic evolution*, and *human activities*, and merging similar micro-scenarios into the five non-reference scenarios listed above.

The results reported hereafter have been obtained by focusing only on the scenario and parametric components of the overall uncertainty.

4 A model uncertainty audit

In this section we present results for maximum dose of the nuclide chain, obtained by summing max dose across neptunium, uranium, and thorium (thus we are working with the sum of the maxes over time, $\max_t[N(t)]+\max_t[U(t)]+\max_t[TH(t)]$).

In the simulations the inputs parameters to GTMCHEM were random draws from uniform or log-uniform distributions, with ranges assigned according to plausible physical values (see Prado et al. (1998) for details).

How much of the overall uncertainty about maximum dose is attributable to scenario uncertainty, and how much to parametric uncertainty? To answer this question, following Draper (1995), we performed a *model uncertainty audit*, in which we partitioned the total variance in max dose into two components, between scenarios and within scenarios, the second of which represents the component of uncertainty arising from lack of perfect knowledge of the scenario-specific parameters. The relevant calculations are based on the double-expectation theorem (e.g., Feller 1971): with y as max dose, and scenario i occurring with probability p_i and leading to estimated mean and standard deviation (SD) of y of $\hat{\mu}_i$ and $\hat{\sigma}_i$, respectively (across the 1000 simulation replications),

$$\begin{array}{rcccccc} \hat{V}(y) & = & V_S[\hat{E}(y|S)] & + & E_S[\hat{V}(y|S)] & = \hat{\sigma}^2 \\ & = & \sum_{i=1}^{k} p_i(\hat{\mu}_i - \hat{\mu})^2 & + & \sum_{i=1}^{k} p_i \hat{\sigma}_i^2 & \\ & = & \begin{pmatrix} \text{between-} \\ \text{scenario} \\ \text{variance} \end{pmatrix} & + & \begin{pmatrix} \text{within-} \\ \text{scenario} \\ \text{variance} \end{pmatrix}, & \end{array} \tag{1}$$

where

$$\hat{E}(y) = E_S[\hat{E}(y|S)] = \sum_{i=1}^{k} p_i \hat{\mu}_i = \hat{\mu}, \tag{2}$$

and S identifies a given scenario.

Table 1 presents the scenario-specific mean and SD estimates, together with three possible vectors of scenario probabilities. We obtained the first of these vectors by expert elicitation of the relative plausibility of the nine micro-scenarios described above, and created the other two, for the purpose of sensitivity analysis, by doubling and halving the non-reference-scenario probabilities in the first vector. Table 2 then applies equations (1, 2) using each of the three scenario probability vectors. It may be seen that the percentage of variance arising from scenario uncertainty is quite stable across the three specifications of scenario probabilities, at about 27% of the total variance. Table 2

Table 1: *Scenario-specific estimated means and standard deviations of max dose, together with three possible sets of scenario probabilities.*

Scenario	Estimated Mean ($\hat{\mu}_i$)	Estimated SD ($\hat{\sigma}_i$)	Scenario Probabilities (p_i) 1	2	3
REF	1.21e–7	6.25e–7	.90	.80	.95
FP	6.54e–3	1.06e–2	.0225	.045	.01125
AG	8.94e–6	1.91e–5	.0125	.025	.00625
GA	1.20e–9	4.72e–9	.0125	.025	.00625
HDE	3.10e–7	1.53e–6	.02	.04	.01
EIC	1.07e–6	4.46e–6	.0325	.065	.01625

Table 2: *Sensitivity analysis of results as a function of scenario probabilities.*

Summary	Scenario Probabilities 1	2	3
Overall mean max dose $\hat{\mu}$	1.47e–4	2.95e–4	7.38e–5
Overall SD $\hat{\sigma}$	1.86e–3	2.63e–3	1.32e–3
Overall variance $\hat{\sigma}^2$	3.47e–6	6.89e–6	1.74e–6
Between-scenario variance	9.41e–7	1.84e–6	4.76e–7
Within-scenario variance	2.53e–6	5.06e–6	1.26e–6
% of variance between scenarios	27.1	26.7	27.3
$\hat{\mu}/\hat{\mu}_{\text{REF}}$	1218	2436	610
$\hat{\sigma}/\hat{\sigma}_{\text{REF}}$	2980	4201	2110

says that the mean maximum dose of the nuclide chain is 600–2400 times larger when scenario uncertainty is acknowledged than its value under the Reference scenario, and the uncertainty about max dose on the SD scale is 2,000–4,000 times larger.

Figure 1 presents scenario-specific estimated predictive distributions for log maximum dose, and also plots the composite predictive distribution with scenario probability vector 1. The Fast Pathway and Glacial Advance scenarios lead to max dose values which are noticeably higher and lower than the other four scenarios, respectively. Principally because of this, the composite distribution is considerably heavier-tailed than lognormal, in particular including a small but significant contribution of very high doses from scenario FP.

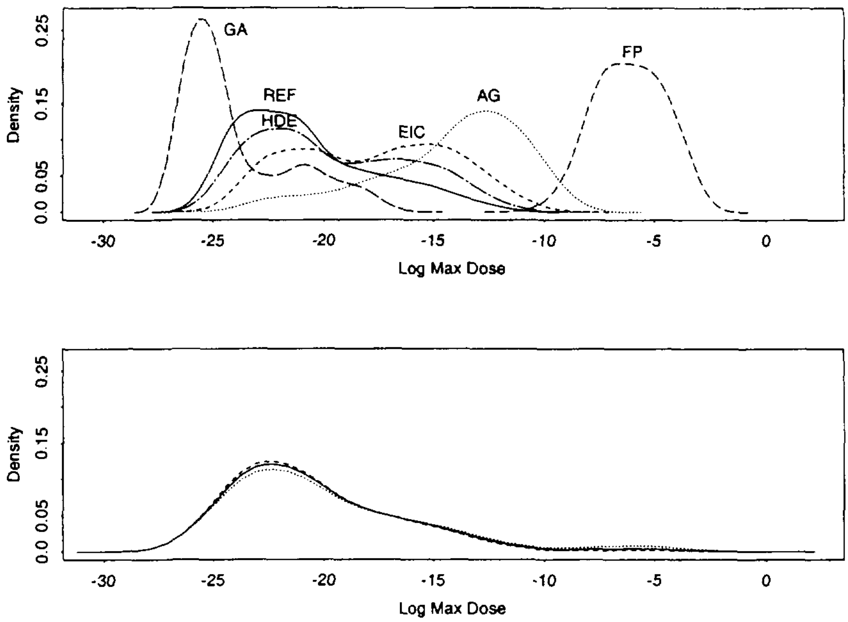

Figure 1: *Scenario-specific predictive distributions for maximum dose (top panel), and composite predictive distribution with scenario probabilities 1–3 (bottom panel). The scenario probability vector again has little effect.*

5 The Extended FAST: An alternative for non-linear sensitivity analysis

Here we describe the results of a sensitivity analysis for radiological dose due to the chain across the six scenarios.

We argue that each uncertain factor has to be described by a pair of indices—first-order and total—and that this kind of representation allows an exhaustive and computationally inexpensive characterization of the system under analysis.

This approach descend from the decomposition of the output variance. According to the analysis of variance, the total output variance V may be uniquely decomposed into orthogonal terms of increasing dimensionality,

$$V = \sum_{i=1}^{k} V_i + \sum_{1 \leq i < j \leq k} V_{ij} + \ldots + V_{12\ldots k}, \tag{3}$$

where k indicates the number of factors and the terms $\{V_{i_1 i_2 \ldots i_s}, i_s \leq k\}$ are called *partial variances*. By dividing these terms by V, *sensitivity indices* (which thus add up to one by definition) can be obtained: $S_{i_1 \ldots i_s} = V_{i_1 \ldots i_s}/V$. Formally, the *total effect index* for factor i is given by

$$S_{Ti} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j < l \neq i} S_{ijl} + \ldots + S_{12\ldots k}. \tag{4}$$

Suitable summary measures can then be obtained by further normalization: $S^*_{Ti} = S_{Ti} / \sum_{j=1}^{k} S_{Tj}$. The S^*_{Ti} are called *total normalized sensitivity indices.*

The pair of first-order/total effect indices for a given factor can be estimated via the same sample with the Extended FAST (Saltelli et al, 1999). The number of samples required for computing the whole set of sensitivity indices by using extended FAST is k. The total number of model evaluations is obtained by multiplying the number of samples needed by the sample size, which is chosen as a function of the desired accuracy for the indices. The number of model evaluations essentially determines the total cost of the analysis: the computational cost of evaluating the sensitivity indices, given the set of model outputs, is negligible.

With an eye to uncertainty analysis, we made FAST computations for the annual radiologic dose due to the chain across all six scenarios in the Level E/G test case, by estimating the first-order and total sensitivity indices for the scenario indicator variable via a set of 5763 model evaluations. The results are expressed as a function of time from 10^3 to $4 \cdot 10^7$ years into the future. The scenario variable interacts with all the factors entering in each and every scenario. In this example the first-order index for the scenario variable is small but its total effect is close to 1! At one level this result is obvious, but it has implications for the theory of sensitivity analysis. It has been argued that when one (group of) factor(s) is important, its first-order effect should be high. This could in some instances allow all the other factors to be fixed without loss of model accuracy (Sobol' 1990). On the other hand, Jansen (1996) argues that the real reduction in model variability that one can achieve by eliminating a factor i (i.e., by considering the i^{th} factor as a perfectly known quantity) is given by its S_{Ti}. In our example, if we were able to eliminate the scenario variable (i.e., by selecting the proper scenario), we would reduce the model variability by around 95% at most of the time points. This is a clear measure of how much the scenario variable influences the output uncertainty. In problem settings where one seeks a group of factors accounting for most of the variance so that the others can be fixed, one should focus on the total effect of the target group, and not on its first-order effect.

6 Discussion

We draw the following conclusions relevant to uncertainty and sensitivity analysis from the GESAMAC study.

- When scenario uncertainty is assessed and propagated along with parametric uncertainty, the component of predictive variance associated with scenario uncertainty may well be 50% or more of the total across the other components. It has been common in the past to ignore this component of uncertainty or to treat it qualitatively; we believe that only through a quantitative approach like the one presented here can the full extent of the relevant uncertainties be appreciated.

- Variance-based sensitivity analyses (Extended FAST in this example) are useful tools for achieving an understanding of the mapping from inputs to outputs in complex simulation environments, where nonlinearities may well be present. These methods are indeed capable of capturing interaction effects, that may be a crucial issue in a risk analysis study.

- Risk assessment is an interesting setting for uncertainty and sensitivity analysis where one might desire to identify input factors governing the risk, as this may provide guidance for mitigation actions; the same can also help to streamline and prioritise R&D work.

Acknowledgments

This work was partially funded under contract FI4W–CT95–0017 (the GESAMAC project) of the European Commission through its R+D program on "Nuclear Fission Safety" (1994–1998).

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