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DISCUSSION OF THE PAPER "THE USE OF CONDITIONAL SIMULATION IN NUCLEAR WASTE SITE PERFORMANCE ASSESSMENT," BY CAROL A. GOTWAY

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DISCUSSION of the paper

"The Use of Conditional Simulation in Nuclear Waste Site Performance Assessment," by Carol A. Gotway

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INTRODUCTION

First, we applaud Dr. Gotway for seeking via her paper to expose a wider audience of statisticians to the many interesting and challenging modeling and statistical problems in the environmental area. This well-written paper effective explains the WIPP and the context of the analysis. Dr. Gotway's paper describes a geostatistical conditional simulation approach combined with deterministic modeling to estimate the cumulative distribution function (cdf) of groundwater travel time (GWTT), information that is needed for estimating the cumulative release of nuclear waste from the repository.

We begin our discussion with comments and questions on modeling aspects of Dr. Gotway's paper. Then we discuss uncertainty and sensitivity analyses and some of the problems inherent with implementing those techniques, including correlations, elicitation of expert opinion, and planning to achieve specified Data Quality Objectives (DQOs).

MODELING

This paper presents the sequential nature of the complex calculations required to predict the performance of a geologic repository. Such a prediction is necessary to obtain regulatory approval for transuranic waste disposal. Dr. Gotway's paper shows the calculations for one part of the process: the groundwater travel time in the Culebra Dolomite from a location above the center of the repository over a distance (unspecified in the paper) outside the boundaries of the current WIPP site.

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Under the current conceptual model for the behavior of the bedded salt in the Salado formation, the only credible potential pathway for the repository contents to reach the Culebra in 10,000 years is through a borehole intrusion into the repository. Transmissivity is clearly an important variable determining the transport of radionuclides in the Culebra. Other major sources of uncertainty include the quantity of radionuclides introduced to the Culebra and the amount of chemical retardation provided by the Culebra to slow the transport of individual constituents. Estimating the transmissivity field is computationally intensive with a 0.5 km grid size (3486 grid elements) from 41 measured values at irregularly-spaced boreholes. Although the emphasis of the paper is on estimating the variogram of the transmissivity measurements, it is interesting to note that the robust estimator of the empirical variogram was not used. Instead, the method of moments estimator was used to provide the "data" for modeling the parametric (exponential) variogram.

The validity of the transmissivity field simulation process (Sections III and IV) is clearly an important topic. It should be possible to check the validity of the generated transmissivity field by comparing the multiple realizations of the transmissivity field to new transmissivity data collected over the site. While collecting new data may be expensive, a confirmation that the simulation procedure provides reasonable transmissivity results would help establish the validity of the GWTT cdf. Of course, the validity of the transfer function and of the GWTT cdf is much more difficult and can be addressed only indirectly by using tools such as uncertainty and sensitivity analyses (discussed later).

The groundwater flow model (equation 5.1) contains several variables, but only permeability (k), which is related to transmissivity (T) and aquifer thickness (b) by $T = bk$, is treated as stochastic for this analysis. Although equation 5.1 is solved for pressure, it must be calibrated to existing pressure measurements that are a function of both time and space. The model calibration procedure is a fascinating statistical problem, showing the complex relationships between the model parameters and measured variables. It is unfortunate that Dr. Gotway did not describe the proposed methodology of LaVenue and Pickens (1992) in more detail, as it is not yet available in the open literature. Presumably, their proposed methodology is based on the inverse methodology developed by Neuman and Yakowitz (1979). We note in passing that Dr. Gotway does not indicate why equation (5.1) was solved using 44 different simulated transmissivity fields. That is, why were 44 runs used?

Regarding the use of conditional simulations, we wonder if it makes sense to force the simulated surface to pass through the original transmissivity data points. That procedure seems to imply the measured data are "true" with no uncertainty. What would be the effect on the predicted GWTT if that restriction were relaxed so that measurement variability and uncertainty were included in the analysis?

UNCERTAINTY AND SENSITIVITY ANALYSIS

In the summary of her paper, Dr. Gotway states that the statistical properties of the procedure in her paper have not been studied. She indicates that future work should include sensitivity analyses, comparison of stochastic simulation algorithms, and evaluations to determine the robustness of methods to departure from key assumptions. We whole heartily agree with the need for such studies, and, in the remainder of this discussion, offer some comments on that topic.

Dr. Gotway outlines a method currently being used to estimate the cdf of GWTT. This method generates realizations of GWTT using a model of the spatial variability of transmissivities and a deterministic transfer function. The cdf is intended to represent the uncertainty of predicted GWTTs obtained using the transfer function. The process used to obtain the cdf is uncertainty analysis (IAEA 1989; Morgan and Henrion 1990). Of course, the estimated cdf itself has uncertainty because of uncertainty about several factors, including the variogram model, the method used to obtain multiple realizations of transmissivities, the deterministic transfer function model, model parameter values, and sampling and measurement errors.

Dr. Gotway does not discuss the model that links GWTT to the quantity of interest, namely the rate that radionuclides are released from the WIPP. Nevertheless, uncertainty in predicted GWTT probably will be a major component of the uncertainty in the predicted release rate. The uncertainty of this rate becomes important if it is large enough for the uncertainty error band around the cdf of release rate to approach or exceed regulatory limits or guidelines (Bingham 1992). In this situation, it is important to determine how much the uncertainty in predicted release rate could be reduced by reducing the uncertainty in the predicted GWTT. Whether it is possible to substantially reduce that uncertainty can be investigated by using sensitivity analysis. This process determines those components of the GWTT model that contribute the most uncertainty to predicted GWTT values. Then, efforts to reduce uncertainty in predicted GWTTs, and consequently in the predicted release rates, can focus on those key sources of uncertainty.

There are several methods of conducting sensitivity analyses, including

- deterministic methods where one or more factors are allowed to vary while other factors are held constant at nominal values
- the standardized partial differential method
- parametric response surface methods, where one or more factors are systematically assigned values according to a design
- probabilistic methods that apply correlation, rank correlation, and regression to the multiple realizations obtained from uncertainty analyses.

Such methods are discussed in, e.g. Morgan and Henrion (1990), Iman and Helton (1985), Iman et al. (1985), and McKay et al. (1992).

Sensitivity analyses using Latin Hypercube sampling and response surface methodologies are a large part of the WIPP Performance Assessment program, although Dr. Gotway does not discuss these analyses. It would be helpful if, in her rejoinder to this discussion, Dr. Gotway would discuss the sensitivity methods being used together with applicable references to their work. One such reference is Helton et al. (1992). Culebra travel time is one of 45 variables used in the sensitivity and uncertainty analyses described in that paper.

CORRELATION

An important part of the procedure discussed in Dr. Gotway's paper is the use of geostatistics to include the spatial correlation structure of transmissivity measurements in the simulation process. Although spatial correlation is certainly an important factor, other types of correlations must also be considered, such as correlations among model parameters and correlations that arise from the structure and interrelationships among model components. With regard to structural correlations, experience has shown (Simpson 1993) the importance of maintaining and propagating structural correlation throughout all model and submodel calculations needed to estimate each realization of the final output. Care must be taken not to lose structural correlation by storing intermediate results as, e.g. a cdf, and then regenerating random realizations from the cdf for use at later stages in the modeling process.

As concerns parameter correlations, a substantial lack of knowledge and data for selecting or estimating the correlations is often the case. In some situations, it may be possible to conduct field studies to obtain the needed information. In other cases, reliance on expert opinion may be the only option.

ELICITATION OF EXPERT OPINION

The elicitation of expert opinion is an extremely important aspect of many uncertainty analyses of deterministic models. Experts are typically needed for several reasons, including developing conceptual and mathematical models, reconstructing important historical events, and developing (encoding) cdfs that characterize lack of knowledge about parameter values. Some recent references on the elicitation of expert opinion are Meyer and Booker (1991), Cooke (1991), Morgan and Henrion (1990), Roberds (1990), Hora and Iman (1989), and Elderkin and Kelly (1990). Although elicitation of expert opinion is clearly an important component of uncertainty and sensitivity analyses, it is appropriate only when relevant data is not available or cannot be obtained by measurement or by searching through historical records. Careful documentation of the elicitation and reasoning processes must be generated.

DATA QUALITY OBJECTIVES

Two problems that must be faced are (1) establishing the acceptable probabilities of making decision errors for the bottom-line decisions, and (2) determining which components of the deterministic and statistical models have uncertainties that will result in unacceptably large decision error rates.

The following questions arise:

- What are the Data Quality Objectives (DQOs)? For example, what levels of accuracy and precision of the cdf of travel time and release rate are required?
- What are the acceptable probabilities of making Type I and Type II decision errors when deciding whether the WIPP can meet EPA regulations?
- What level of effort (measured in dollars and time) is reasonable to expend to reduce decision error rates?

The thought of working backwards from DQOs on performance measures to data needs when complicated models are present may boggle the mind. However, a successful approach could include the use of uncertainty and sensitivity analyses to determine the components that contribute large uncertainties to predictions. Then, setting DQOs that must or can be achieved for the cdf of GWTT and the important components could lead to better assessments of needed dollar and time resources.

ADDITIONAL REFERENCES

Bingham, F.W. (1992). *Is it Possible to Demonstrate Compliance with the Regulations for High-Level-Waste Repositories?*, SAND--92-2335C, Sandia National Laboratories, Albuquerque, New Mexico.

Cooke, R.M. (1991). *Experts in Uncertainty, Opinion and Subjective Probability in Science*, Oxford University Press, New York.

Elderkin, C.E. and Kelly, G.N. (editors) (1990). *Proceedings of the CEC/USDOE Workshop on Uncertainty Analysis*, PNL-SA-18372, Pacific Northwest Laboratory, Richland, Washington.

Helton, J.C., Garner, J.W., Rechard, R.P., Rudeen, D.K., and Swift, P.N.. (1992). *Preliminary Comparison with 40 CFR Part 191, Subpart B for the Waste Isolation Pilot Plant, December 1991/ Volume 4: Uncertainty and Sensitivity Analysis Results*. SAND91-0893/4. Sandia National Laboratories, Albuquerque, New Mexico.

Hora, S.C. and Iman, R.L. (1989). "Expert Opinion in Risk Analysis: The NUREG-1150 Methodology," *Nuclear Science and Engineering* 102:323-331.

IAEA (1989). *Evaluating the Reliability of Predictions Made Using Environmental Transfer Models*, Safety Series No. 100, International Atomic Energy Agency, Vienna, Austria.

Iman, R.L. and Helton, F.C. (1985) *A Comparison of Uncertainty and Sensitivity Analysis Techniques for Computer Models*, NUREG/CR/3904, Nuclear Regulatory Commission, Washington, D.C.

Iman, R.L., Shortencarier, M.J., and Johnson, J.D. (1985). *A Fortran 77 Program and User's Guide for Calculation of Partial Correlation and Standardized Regression Coefficients*, NUREG/CR-4122, Sandia National Laboratories, Albuquerque, New Mexico.

McKay, M.D., Beckman, R.J., Moore, L.M., and Picard, R.R. (1992). "An Alternative View of Sensitivity in the Analysis of Computer Codes," *Proceedings of the Section on Physical and Engineering Sciences of the American Statistical Association*, pp. 87-92.

Meyer, M.A. and Booker, J.M. (1991). *Eliciting and Analyzing Expert Judgement, A Practical Guide*, Academic Press, New York.

Morgan, M.G. and Henrion, M. (1990). *Uncertainty, A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*, Cambridge University Press, New York.

Roberds, W.J. (1990). "Methods for Developing Defensible Subjective Probability Assessments," *Transportation Research Record*, No. 1288, Transportation Research Board, National Research council, Washington, D.C.

Simpson, J.C. (1993). *Effects of the Loss of Correlation Structure on Phase I Dose Estimates*, PNWD-7638 HEDR, Hanford Environmental Dose Reconstruction Project, Battelle, Pacific Northwest Laboratories, Richland, Washington.

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