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STOCHASTIC ANALYSIS OF CONTAMINANT TRANSPORT

Final Report

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ABSTRACT

A reliability algorithm is used to develop probabilistic (stochastic) models of contaminant transport in porous media. The models are based on advective-dispersive transport equations, and utilize the reliability algorithm with existing one- and two-dimensional analytical and numerical solutions. Uncertain variables in the models include: groundwater flow velocity (or permeability in the numerical model), dispersivity, diffusion coefficient, bulk density, porosity, and solute distribution coefficient. Each uncertain variable is assigned a mean, covariance, and marginal distribution. The models yield an estimate of the probability that the contaminant concentration will equal or exceed a target concentration at a selected location and time. The models also yield probabilistic sensitivity measures which identify those uncertain variables with most influence on the probabilistic outcome.

The objective is to examine the basic behavior and develop general conclusions regarding transport under uncertain conditions as modeled using a reliability approach. A wide range of statistical input and problem assumptions is assumed for some hypothetical problems. Results indicate that simplification of the analysis is possible by a preliminary determination of probabilistic sensitivity measures. Those variables with low sensitivity can effectively be treated as deterministic constants. In analytical models, flow velocity is usually the most important uncertain variable; dispersivity can often be treated as a deterministic constant. Numerical model results, however, indicate dispersivity has more probabilistic influence than permeability if dispersivity is treated as a single global variable while the permeability is treated as a discretized variable. In reactive transport, the bulk density, fluid density, and distribution coefficient are always very important uncertain variables.

INTRODUCTION

This report provides a comprehensive summary of research progress and results concerning the project "Stochastic Analysis of Contaminant Transport" -- Dr. Jeffrey D. Cawlfield, Principal Investigator. This project has been supported by the U.S. Department of Energy, Office of Energy Research, Ecological Research Division, Subsurface Science Program. Program manager is Dr. Frank Wobber.

The report includes a summary discussion of Goals and Objectives, Methodology, Results, and Conclusions. Appendix No. 1 is a listing of reports, conference proceedings, and presentations resulting from the research project. Appendix No. 2 includes copies of three manuscripts which have been prepared for journal or conference presentation; the reader is referred to these manuscripts for details of literature review, theoretical development, model construction and coding, and specific results.

GOALS AND OBJECTIVES

The research project was focused on development of one- and two-dimensional probabilistic (stochastic) models of contaminant transport in porous media. The reliability algorithm, which has been used for years in structural mechanics, is of particular interest because it is often more efficient than other probabilistic methods for estimating a probability measure and, perhaps most importantly, for evaluating probabilistic sensitivity measures. Models were developed by coupling a reliability algorithm with existing analytical and numerical solutions of the advective-dispersive solute transport equations. The goal was to study the basic behavior of solute transport under conditions of uncertainty as modeled in a probabilistic framework. Specific objectives are as follows:

- Construct one- and two-dimensional probabilistic analytical models and apply these models to typical simplistic flow regimes which are often modeled using analytical solutions.

- Conduct a literature search, interact with other DOE researchers and scientists, in order to develop a range of typical statistical characteristics for the selected uncertain variables.

- Evaluate the importance of each uncertain variable, the magnitude of uncertainty, correlation between variables, and the marginal PDF.

- Emphasize the utility of the probabilistic alpha and gamma sensitivity measures, as commonly evaluated during reliability analyses.

- Building upon the probabilistic analytical results, develop a probabilistic numerical model by coupling the reliability algorithm with an existing two-dimensional finite element model of solute transport. Examine the issues as stated above with respect to uncertain variable importance. Most importantly, confirm or reject preliminary conclusions from analytical results and investigate the importance of spatial correlation between permeability.

METHODOLOGY

The investigative procedure is straightforward:

- construct the probabilistic analytical models,

- select some typical hypothetical problems,

- apply the models to the example problems,

- repeat the analysis over a wide range of statistical input and problem assumptions,

- focus on the interesting results and critical issues brought out by the analyses, especially with respect to practical modeling in a risk/cost/benefit scenario.

- repeat the procedure for probabilistic numerical model, with particular emphasis on spatial correlation and verification of interesting results from the analytical studies.

RESULTS

During the first twelve months or so of the project, the emphasis was placed on developing one- and two-dimensional probabilistic analytical models of transport. Theoretical background, model development, results and conclusions are discussed in some detail in Cawlfield and Wu (1992c, in review) and Wu and Cawlfield (1992a, in press), both contained in Appendix No. 2.

Cawlfield and Wu (1992c, in review) discusses the one-dimensional probabilistic transport results for both relatively low flow velocity and relatively high flow velocity regimes. Both reactive and non-reactive transport is considered. Although based on rather simplistic problem geometry and boundary conditions, the analytical models lend insight into basic behavior and potential limitations of the approach. Major conclusions are that the flow velocity is usually the most important uncertain variable within a probabilistic framework. When the uncertainty of diffusion coefficient is much higher than flow velocity, diffusion coefficient may become as important or more important to the probabilistic outcome. Dispersivity does not seem to be an important uncertain variable in the analytical solutions and, therefore, can be treated as a deterministic constant. In reactive transport, the bulk density, porosity, and distribution coefficient are all very important uncertain variables. Correlation between variables can be a critical issue, as can marginal PDF, but only for variables with relatively high sensitivity values.

Wu and Cawlfield (1992a, in press) discuss two-dimensional probabilistic analytical results. The one-dimensional conclusions were confirmed (for analytical models ONLY), and two-dimensional effects were seen to be as expected: x and y components of flow velocity dominated the probabilistic outcome in most cases. One very interesting result described in Wu and Cawlfield (1992a, in press) is the progressive decline of importance in bulk density, porosity and distribution coefficient (the reaction terms) as the transport event continues in time. For a target concentration at a selected location and relatively long time after transport begins, there will be cases where the reaction terms have negligible effect on the probabilistic outcome and can, therefore, be treated as deterministic constants. Such a simplification of the problem for certain conditions would offer a tremendous savings in time and effort because the statistical characteristics of the reaction terms would not be needed.

The numerical probabilistic model focused on discretizing the uncertain permeability in space and studying the effect of spatial correlation between permeability. A short conference proceeding paper is attached in Appendix No. 2 (Cawlfield and Wu, 1992b) which describes the basic approach, the numerical solution model used, and some of the major results. A more detailed manuscript is being prepared for submittal later in 1992.

The numerical results offer some surprises. For example, dispersivity is modeled as a single global uncertain variable which is statistically homogenous over the entire finite element grid. Permeability is modeled as a discretized uncertain variable with mean, marginal PDF, and covariance defined element by element. Within such a structure, the probabilistic sensitivity measure indicates the dispersivity is the most important uncertain variable to the probabilistic outcome. Recall that dispersivity was considered of low importance in the probabilistic analytical results and, therefore, could be treated as a deterministic constant. Even in reactive transport, the dispersivity, when treated as a global variable, is one of the most important uncertain parameters. Why is there this discrepancy? Further modeling is needed, but the evidence indicates that the probabilistic sensitivities are a function of spatial discretization: if dispersivity is modeled as a elemental or nodal variable it is expected that the probabilistic sensitivity measures would decrease dramatically. In the analytical models, all variables were effectively global, with a single uncertain variable over the entire region. Since permeability is discretized (in our examples there were 320 elements; therefore, 320 individual uncertain permeability variables) the probabilistic sensitivity for any one of those variables is relatively low.

By looking only at probabilistic sensitivity for the discretized variables, the analyst can obtain some very valuable information about the spatial location of the most important variables. Cawlfield and Wu (1992b) show an example grid with the high sensitivity variables identified. Such information will prove invaluable for designing field sampling programs or for identifying locations for additional sampling. Spatial correlation between the elemental permeability values is shown to be of relatively low importance with regard to the probabilistic outcome for the examples studied, although this should not be construed as an exhaustive statement. Further studies on more complex numerical problems is needed to delineate when and where spatial correlation has maximum and minimum impact.

More efficient means for calculating the sensitivity measures are needed in numerical based solution procedures. When 100's of uncertain variables are included, the common approach of calculating finite divided differences during the sensitivity calculation is computationally inefficient. Adjoint methods, programmed sensitivity calculations, and direct differentiation offer the potential for efficient calculation. It is recommended that additional work with numerical probabilistic methods be focused in this direction.

CONCLUSIONS

The reliability algorithm provides an attractive alternative in many situations to other probabilistic methods. It directly calculates a probability estimate and probabilistic sensitivity information. The probabilistic sensitivity information can be used to greatly simplify a probabilistic analysis; further, such information can be used to optimize field and laboratory sampling and analysis.

The research conducted under this project has shown that the reliability algorithm is effective and of great practical use. There are limitations, however, such as the computational burden of evaluating sensitivity measures for numerical based solutions when 100's of uncertain variables are included. This area needs further research to improve the efficiency. The reliability probability measures are approximate and, in some cases, the approximation can be quite rough. However, the sensitivity information will still be of practical use and more accurate second-order approximations of the probability measure are available at additional computational cost.

Results have indicated that the discretization of uncertain variables has a great effect on the general conclusions regarding the basic behavior of the transport process under conditions of uncertainty. Dispersivity is shown to have little influence on the probabilistic outcome in analytical based solutions; however, in the numerical studies where dispersivity is a single global variable, it can dominate the outcome. Further research is needed to clarify this quandary, but it is expected that if dispersivity is treated as a discretized variable its relative importance will diminish significantly.

Flow velocity and reaction terms are always important -- the most important of these uncertain variables will be dictated by relative magnitude of uncertainty. Correlation between these variables is also important. Surprisingly, autocorrelation between element permeabilities in the numerical studies did not have much impact on the probabilistic outcome. Further studies on autocorrelation are needed to refine this preliminary conclusion.

The goals and objectives of the original research plan have been addressed and completed. A proposal for further work has been submitted and is currently in review. The proposal includes focus on probabilistic sensitivity measures for evaluation of spatial correlation, more efficient calculation of sensitivity terms, and a scheme for probabilistic updating using measurements of the performance criterion after the initial analysis.

APPENDIX NO. 1

Publications, Conference Proceedings, and Presentations Resulting From This Grant

Cawlfield, J.D., and Ming-Chee Wu, "Critical issues related to a combined probabilistic/numerical analysis of contaminant transport in porous media", ASCE Specialty Conference on Probabilistic Mechanics, and Structural and Geotechnical Reliability, July 8-10, 1992, (in press).

Wu, Ming-Chee, and J.D. Cawlfield, "Probabilistic analysis for contaminant transport in porous media with reliability analysis algorithm", Sixth International Symposium on Stochastic Hydraulics, May 18-20, Taipei, Taiwan, (in preparation).

Cawlfield, J.D., and Ming-Chee Wu, "Probabilistic analysis for one-dimensional reactive transport in porous media", submitted to Water Resources Research, 1992 (in review).

Wu, Ming-Chee, and J.D. Cawlfield, "Probabilistic sensitivity and modeling of two-dimensional transport in porous media", Stochastic Hydrology and Hydraulics, 1992, in press.

Cawlfield, J.D., "Evaluating probability measures related to subsurface flow and transport: Overview of technical considerations and modeling philosophy", 1991 International Symposium on Groundwater, ASCE, Proceedings, Gerard P. Lennon (ed.), 1991.

Wu, Ming-Chee, and J.D. Cawlfield, "Sensitivity of stochastic transport solution to probability density functional form and variability for uncertain flow velocity, diffusion, and dispersivity", (abs.), American Geophysical Union, Spring Meeting, Baltimore, May-June, 1990.

Wu, Ming-Chee, and J.D. Cawlfield, "First-order approach for probabilistic analysis of contaminant transport in porous media", (abs.), Association of Engineering Geologists, Program and Abstracts, 32nd Annual Meeting, Vail, Colorado, 1989.

Cawlfield, J.D., "A general approach for evaluating risk due to groundwater flow, contaminant transport and geologic hazards", (abs.), Transactions of the Missouri Academy of Science, 1989.

APPENDIX NO. 2

Copies of the following manuscripts:

Wu, M.-C., and J.D. Cawlfield, Probabilistic sensitivity and modeling of two-dimensional transport in porous media, Stochastic Hydrology and Hydraulics, 1992a, (in press).

Cawlfield, J.D., and M.-C. Wu, Critical issues related to a combined probabilistic/numerical analysis of contaminant transport in porous media, ASCE Specialty Conference on Probabilistic Mechanics, and Structural and Geotechnical Reliability, July 8-10, 1992b (in press).

Cawlfield, J.D., and M.-C. Wu, Probabilistic analysis for one-dimensional reactive transport in porous media, Water Resour. Res., 1992c, (in review).

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