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Uncertainty Analysis with Site-Specific Groundwater Models: Experiences and Observations

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ABSTRACT

Groundwater flow and transport predictions are a major component of remedial action evaluations for contaminated groundwater at the Savannah River Site. Because all groundwater modeling results are subject to uncertainty from various causes; quantification of the level of uncertainty in the modeling predictions is beneficial to project decision makers. Complex site-specific models present formidable challenges for implementing an uncertainty analysis.

We present an overview of our experiences in conducting uncertainty analyses using the Monte Carlo method on two MODFLOW/MODPATH/MT3DMS groundwater flow and transport models in the reactor areas of the Savannah River Site. Each analysis required extensive computational resources, which were managed using pseudo-distributed computing with an Excel-based application on desktop computers. The Monte Carlo results were filtered using flow model calibration targets.

The C-Area Groundwater Operable Unit uncertainty analysis focused on TCE discharge to the model boundary streams and used a nine layer (56,682 cell) finite difference grid with 5,000 eight-parameter-realization sets – 926 of which met calibration filtering requirements. The uncertainty analysis for the R-Reactor Seepage Basin Operable Unit focused on strontium-90 transport and used a 20 layer (214,200 cell) finite difference grid with 18,000 nineteen-parameter-realization sets – 1729 of which met calibration filtering requirements.

INTRODUCTION

It is widely known that any prediction of natural processes, particularly those involving the subsurface, has numerous sources of uncertainty. Hydrogeologic heterogeneity, modeling and conceptual simplifications, and sampling distribution and frequency all contribute to modeling uncertainty (NRC 1993, USEPA 1999, Zimmermann 2000). In environmental restoration evaluations at the Savannah River Site (SRS), project uncertainty, and therefore risk, is typically managed by using conservative model parameters and assumptions to arrive at near upper bound predictions. Recently, government agencies and stakeholders have acknowledged the need to manage the risk more reasonably and quantitatively (Paté-Cornell 1996).

The purpose of SRS uncertainty analyses is to quantify the uncertainty of the calibrated model results due to uncertainty in model parameters. An uncertainty analysis is accomplished by simultaneously varying multiple parameters and evaluating the results that preserve calibration. The analysis method used for SRS groundwater modeling is the traditional Monte Carlo technique (Copt and Findikakis 2000, Parker and Islam 2000). Because of the computational requirements, Monte Carlo is not often used with complex models of environmental systems (Isukapalli et al. 1998), even though it may be the only method capable of estimating uncertainty in highly non-linear and/or complex systems (Warwick and Cale 1986, Bright et al. 2002). Because the Monte Carlo technique allows complete definition of the range of each uncertain parameter and is straightforward to implement, even though it requires significant computational effort (Zio and Apostolakis 1999), it is the current preferred method for quantifying model uncertainty at SRS.

The SRS borders the Savannah River in west-central South Carolina (Figure 1). The 300 mi² site is underlain by Atlantic Coastal Plain sediments which thicken to the southeast. These sediments vary in thickness from 600 to 1200 ft across the site and consist of interbedded sands, silts, and clays, with some gravel and carbonate deposits (Aadland et al. 1995). Due to the complexity of the depositional

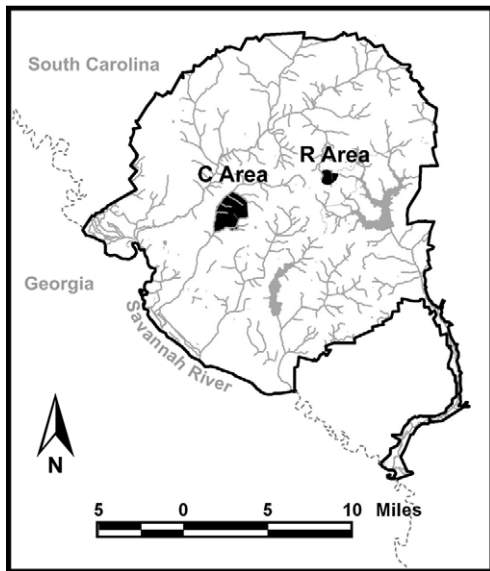


Figure 1. Location of example project areas at the Savannah River Site.

environments that existed in this area (fluvial and near shore marine), sandy aquifer zones and clay/silt layers that act as confining units can vary widely in composition and pinch out over relatively short distances. Consequently a system of aquifers, intermingled with aquitards/aquicludes, exists which tends to vary in hydraulic conductivity and contaminant transport potential.

In this paper, we present our observations and experiences in performing uncertainty analysis for two SRS projects (see Figure 1). The C-Area Groundwater (CGW) project included a trichloroethene (TCE) plume and two stream receptors. The uncertainty analysis assisted in the decision against the need for an early action and the acquisition of additional characterization data. The R-Area Reactor Seepage Basins (RRSB) project focused on a relatively stationary strontium-90 (Sr-90) plume. The analysis provides an understanding of expected results for a monitored natural attenuation remedy. Detailed model domains for each project are given in Figure 2.

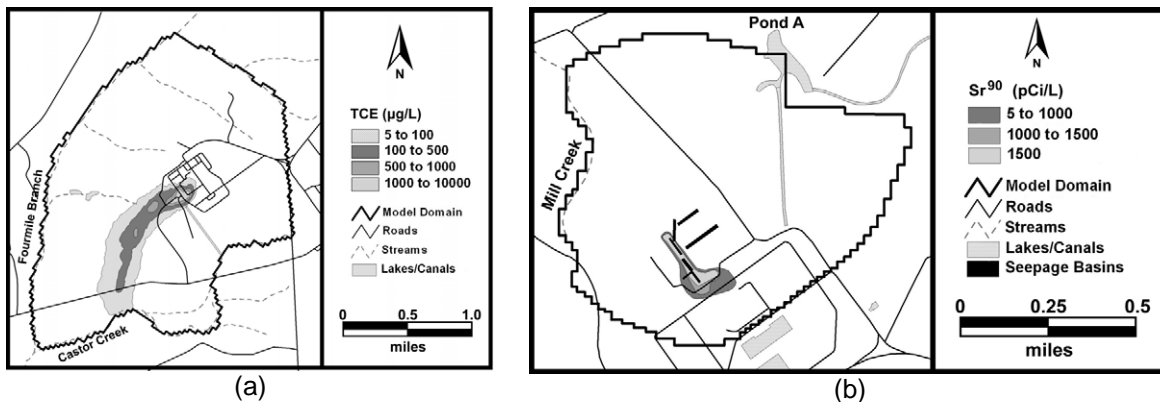


Figure 2. Model domains: (a) C-Area Groundwater, (b) R-Area Reactor Seepage Basins

DISCUSSION

Monte Carlo Methodology

The basic steps for an uncertainty analysis have been defined by many researchers and practitioners (Carroll and Warwick 2001, USEPA 1997, Zio and Apostolakis 1999). In our work, we generate a group of random parameter sets that match the desired probability distributions for the uncertain parameters. Then we execute multiple realizations using Excel and a custom driver program written in Visual Basic. Because the random parameter sets have been predefined, we are able to manually distribute the realization calculations to different computers (desktop PCs), and manually recombine the results. Each realization involves evaluating a random parameter set as follows: 1) change the model input files to reflect the new parameter values being evaluated; 2) run MODFLOW; 3) if MODFLOW converged, check the calibration; 4) if the MODFLOW solution met the filtering requirements, run MODPATH and record the required results; 5) run MT3DMS and check the mass balance; and 6) if the MT3DMS solution met the mass balance requirements, record the required results. After the realizations are complete, we analyze the results and calculate the desired uncertainty results (confidence intervals, etc.).

According to Vose (1996), the cardinal rule of risk analysis modeling is that “Every iteration (realization) of a risk analysis model must represent a scenario that could physically occur.” For groundwater modeling, the realistic plausibility of each realization can be determined by evaluating calibration criteria – if a realization does not meet calibration criteria it can be considered unrealistic and should not be included in the uncertainty analysis results. The calibration criteria for the uncertainty analysis should be similar to the criteria used in the original model calibration. Target values and acceptable ranges for calibration statistics, individual heads, and fluxes are defined to ensure a representative and spatially distributed target set. Although it would be possible to incorporate transport model calibration criteria into the filtering process, the quality and level of information to establish concentration targets were not available for the two example projects discussed in this paper.

Simple head and flux target filter criteria were used in the CGW project. In the RRSB project, four flow calibration filter criteria were used: root mean squared error, mean absolute error, mean error, and percentage of wells within three feet of target values. There were no flux targets available for the RRSB project.

C-Area Groundwater Project Analysis

The CGW project uncertainty analysis focused on total TCE flux to streams and consisted of parameter uncertainty for eight parameters including horizontal and vertical hydraulic conductivities (by model layer), porosity, recharge, and dispersivity. Other project uncertainties (such as source location and future source loading) were handled with conservative assumptions. The nine-layer flow and transport model consisted of a computational grid with 56,682 total cells and a transport simulation time of 50 years. A total of 5,000 Monte Carlo realizations were performed, with 926 passing the head and flux filter. An analysis of cumulative statistics of the computed TCE flux to streams showed stability after a few hundred realizations, indicating adequate realizations for the analysis.

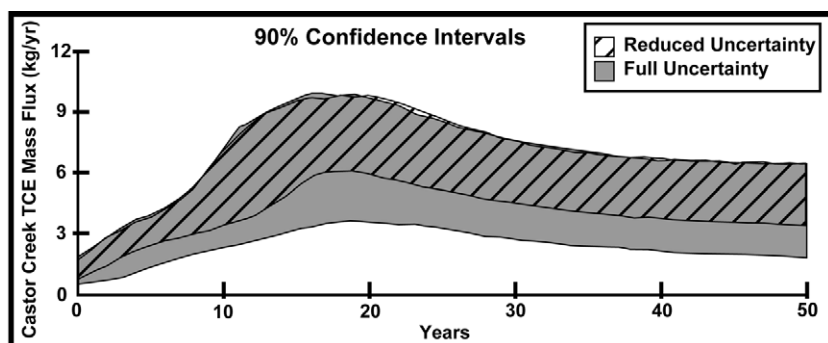


Figure 3. CGW TCE flux to stream results with full uncertainty, and with reduced uncertainty.

The predicted uncertainty in TCE fluxes to the stream receptors (discharge locations) were calculated, with the major stream receptor results shown in Figure 3. By examining the relationship between parameter values and resulting TCE flux to streams, we determined that the horizontal hydraulic conductivity for a middle aquifer layer was highly correlated to contaminant flux.

To explore the impact (i.e., benefit) of additional characterization information for this parameter, the uncertainty analysis was re-run without that parameter's uncertainty. The TCE flux results from this reduced uncertainty scenario are also shown in Figure 3, and indicate a relatively minor uncertainty reduction.

The uncertainty of the impact of a remedial alternative remedy was also calculated by running the 926 filtered realizations with the remedy, then subtracting the calculated TCE flux to streams from the “basecase” predictions – realization by realization, ensuring the comparison was based on equivalent parameters. The results indicated that the impact of the remedy was highly uncertain.

R-Area Reactor Seepage Basins Project Analysis

The RRSB project uncertainty analysis focused on the fate and transport of a Sr-90 plume and consisted of parameter uncertainty for nineteen parameters including horizontal and vertical hydraulic conductivities

(by model zones), porosity, recharge, sorption coefficient, dispersivity, and source concentration. As with the CGW project, other project uncertainties were managed with conservative assumptions. The twenty-layer flow and transport model consisted of a computational grid with 214,200 total cells and a transport simulation time of 200 years. A total of 18,000 Monte Carlo realizations were attempted, with 1,729 passing the head calibration filters. An analysis of the monitoring well Sr-90 activity concentrations showed stable cumulative statistics on the computed confidence intervals after approximately 1,500 realizations, indicating adequate realizations for the analysis. In addition to this analysis group, the uncertainty analysis was repeated with a verification group, an independent set of 18,000 realizations. As shown in Figure 4, the results from the two groups had an acceptable match.

The uncertainty of monitoring well Sr-90 concentrations was calculated for existing and proposed monitoring well locations. Figure 4 gives the resulting 90% confidence interval (5 to 95% confidence) for a select number of wells.

The Sr-90 plume did not reach the model boundaries in any of the 1,729 filtered realizations (due to high sorption and low flow rates). Because of project concerns, the potential model discharge locations were calculated using particle tracking from source locations. None of the particles exited the model at surface cells.

A secondary part of the RRSB project was to optimize the monitoring network with respect to uncertainty. The average time of flow from source cells (based on particle tracking), the number of realizations which exceeded defined concentration limits at anytime during the simulation (based on transport simulations), and the number of realizations where flow from source cells intersected with the cells of interest (based on particle tracking) were determined and/or calculated at potential monitoring well locations. These values were related to the probability of a potential detection, the certainty of detection, and the early detection probability, respectively; and were included in an objective function as part of the optimization determination.

General Observations

In addition to the project specific results, a number of general observations were made as a result of performing these two uncertainty analyses.

During development of the first version of our driver code, we elected to recompile the MODFLOW and MT3DMS source code

distributed with the Groundwater Modeling System (BYU 1999) to eliminate seemingly trivial graphical user interface calls. After running the analysis, we discovered that not all realizations performed as expected (see Figure 5 and compare y-axis scale of Figure 3). Detailed examination of the individual highly-abnormal realizations showed unexplainable occurrences such as sources turning off and on during the simulation, boundary cells creating mass, etc. A majority of the realizations, however,

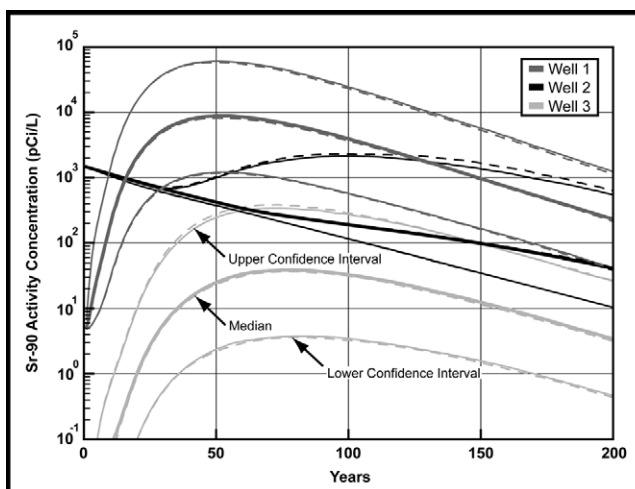


Figure 4. Select RRSB project monitoring well confidence intervals for analysis group (solid lines) and verification group (dashed lines).

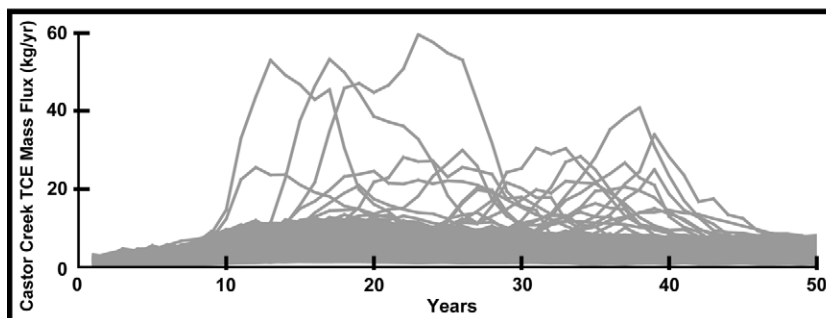


Figure 5. Individual realization results for CGW TCE flux to stream with recompiled code.

performed without any problems. Although the exact cause of the problems with the recompiled code was never determined, we suspected that there were array reference issues introduced with the recompiling. Based on this experience, our more recent analyses do not use recompiled model code and extensive code verification tests are performed.

A limited sensitivity analysis was performed for each project to assess the effect of different parameter distributions and different filter criteria. In the case of the CGW project, altering the distribution type of the primary uncertain parameter (i.e., that parameter that showed the greatest correlation with output results) resulted in no appreciable difference in computed confidence intervals for TCE flux to streams. In the case of the RRSB project, varying the filter criteria caused only a slight impact on resulting monitoring well confidence intervals.

SUMMARY

MODFLOW, MODPATH, and MT3DMS were successfully used to perform uncertainty analyses for two large, complex flow and transport models of shallow aquifer systems using a Monte Carlo approach. The analyses were both successful at assisting project decision makers in managing uncertainty. Based on our experience, we expect future analyses to include further sensitivity analyses on distributions and filter criteria, incorporation of additional types of uncertainty (boundary conditions), and determination of a transport-based calibration filter.

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