Calibration and Reliability in Groundwater Modelling: From Uncertainty to Decision Making
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Los Alamos National Laboratory's risk-based decision analysis for groundwater remediation and monitoring

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Abstract Contaminant transport models can provide valuable information for decisions regarding environmental management. When coupled with quantitative uncertainty, sensitivity, and economic-worth analyses, contaminant transport models can be used to optimize overall performance of an environmental management system. This paper describes a risk-informed decision process developed and applied at Los Alamos National Laboratory in New Mexico, USA, to optimize the management of groundwater-protection program resources. A separate publication (Vesselinov & Birdsell, 2005) describes the groundwater transport model developed to assess uncertainty in this application, while this paper focuses on the decision analysis model developed to manage that uncertainty.

Keywords decision analysis; environmental restoration; groundwater; Monte Carlo analysis; sensitivity analysis; simulation; uncertainty analysis

INTRODUCTION

Background

Los Alamos National Laboratory (LANL) occupies 43 square-miles (110 km^2) in north-central New Mexico, USA. LANL's operation over the past 60 years has resulted in more than 2000 contaminated or potentially contaminated sites that require investigation and possible clean up by LANL's Environmental Restoration (ER) program. Even with this large number of sites, releases to the environment have been minimal and there are no known human exposures to LANL contamination. The reason for the combination of a large number of sites and few serious releases is a semiarid climate, large depth to groundwater (approximately 700–900 feet, 210–270 m, below ground surface), and distance to the nearest water supply wells. Therefore, the major environmental concern is the potential migration of contaminants from the land surface through the vadose zone, into the regional aquifer and to supply wells.

This paper describes a risk-informed decision support process, herein referred to as the LANL Decision Support Process (LANL DSP), that has been developed and implemented to expedite site characterization and clean up. This paper discusses the overall decision analysis process. An application of this process is described in Hollis *et al.* (2005).

Definitions and philosophy

Risk in the general context of groundwater restoration in the United States is usually defined as the likelihood that a person will die due to cancer associated with ingesting water containing a specified concentration of a contaminant. The uncertainty addressed by this definition is in the cause and effect relationship between a potential concentration and a specific health effect—death by cancer. Herein, this risk is referred to as "the risk after exposure." The LANL DSP includes the uncertainty in the estimated concentration used to calculate the risk after exposure. Uncertainty in estimated concentrations arises from uncertainty in the models and parameters that describe source terms and groundwater flow and transport. Herein, the likelihood of being exposed to a specific concentration is labelled "the risk of exposure." The LANL DSP combines both the calculated risk of exposure with the risk after exposure for carcinogens, health indices for non-carcinogens, and dose for radioactive contaminants to arrive at a more complete definition of risk.

Next, we recognize, as did Kaplan & Garrick (1981), that risk ... "*is a subjective thing—it depends upon who is looking. ... risk depends upon what you do and what you know and what you do not know.*" The fact that risk is dependent on who is doing the assessment and who defines the state of knowledge that forms the basis for the risk assessment, is especially important in the contentious environment surrounding environmental contamination. Recognizing this, the LANL DSP strives to include regulators and stakeholders in virtually every step of the risk assessment and decision analysis process, from defining conceptual models and parameter distributions to recommendations for site clean-up.

Finally, the explicit goal of the overall risk-based decision analysis is to proceed to a risk management action at the earliest possible time. In this regard, the LANL DSP realizes that scientific uncertainty will always exist and therefore, the LANL DSP quantifies and propagates all scientific uncertainties to identify and focus on the subset of scientific uncertainties that impact decision making.

RISK-INFORMED DECISION SUPPORT PROCESS

Defining risk-management alternatives

The LANL DSP begins with the end in mind by defining the set of activities that can be undertaken to reduce risk at a specific site. In general, these risk management activities include source control, remediation, monitoring, characterization, research, and land use control.

Defining goals and acceptable uncertainty

The overall goal of the LANL ER project is to protect human health and the environment. To proceed with decision-making, these general goals must become specific, quantified, and measurable. The following goals are defined consistent with US EPA regulations: (a) a dose of less than 4 mrem $year^{-1}$ for radionuclides (EPA, 2003); (b) a Hazard Index (HI) of less than 1.0 for toxic chemicals (EPA, 2000); and (c) an excess incremental cancer probability of less than 1-in-100 000 for carcinogenic non-radiological chemicals.

Simulations have shown that peak concentrations occur within 1000 years in the future. Therefore, the timeframe of concern is set as 1000 years. In addition to defining goals and timeframes, acceptable uncertainty in meeting these goals must be defined at the outset of the process. LANL is currently utilizing a 95% confidence level in meeting the above stated goals.

Defining the state of knowledge used in risk assessment

Currently there are no exposures to LANL contaminants in groundwater. Risks are in the future and estimated by simulations of contaminant migration through the vadose zone and the regional aquifer to water supply wells. These calculations are based on knowledge about the source term, geohydrological conditions, and contaminant properties. Such factors are: (a) uncertain; and (b) a function of who is defining them. Thus, the LANL DSP process attempts to define a comprehensive state of knowledge among all involved parties. The goal is not consensus about what is known or believed about the site. Instead, the goal is to define ranges of parameter values and assumptions (conceptual models) held by all stakeholders (including LANL scientists) that are not inconsistent with available data or science. The LANL DSP then defines probability density functions (PDFs) that represent the range of opinion/belief and sets of conceptual models arising from differing assumptions. All potential parameter values and sets of assumptions (conceptual models) are propagated through groundwater flow and transport simulations and the results are passed on to the next step in the decision process. Inherent in this process is the recognition that different parameter values or assumptions may or may not lead to different risk management decisions.

Groundwater flow and transport simulations

Hollis *et al.* (2005) and Vesselinov & Birdsell (2005) describe details of the vadose zone and regional aquifer flow and transport calculations. In this paper, it is sufficient to note that 1000 Monte Carlo simulations based on Latin Hypercube Sampling (Wyss & Jorgensen, 1998) are performed resulting in equally likely sets of parameter input and model output for each conceptual model. Sensitivity analysis has shown that 1000 simulations are adequate for covering the range of parameter input values. These calculations form the basis for the baseline risk assessment and further decision analysis.

Baseline risk calculation

Concentrations for each conceptual model at all supply wells are converted to dose, HI, or cancer-risk values by employing exposure assumptions defined by the US EPA.

Exposure assumptions include a 70 kg person ingesting 2 L day^{-1} of water for 70 years and include the same reference dose factors that EPA uses in setting the maximum concentration limits (MCLs) for groundwater (EPA, 2003). The maximum 70-year averaged concentration at every water supply well is found for each 1000 year simulation. Because there are 1000 simulations, this search yields 1000 HI, dose, and/or cancer-risk values for each conceptual model at each supply well. Next, these values are arranged from largest to smallest and a complementary cumulative distribution function is developed for each of the supply wells. At this stage, each simulation result has the same probability of occurrence, 1/1000. Alternative weighting, based on how well simulation results match monitoring data, has also been developed and tested. In the following figure, equal weighted perchlorate HI values are displayed for one conceptual model and three production wells.

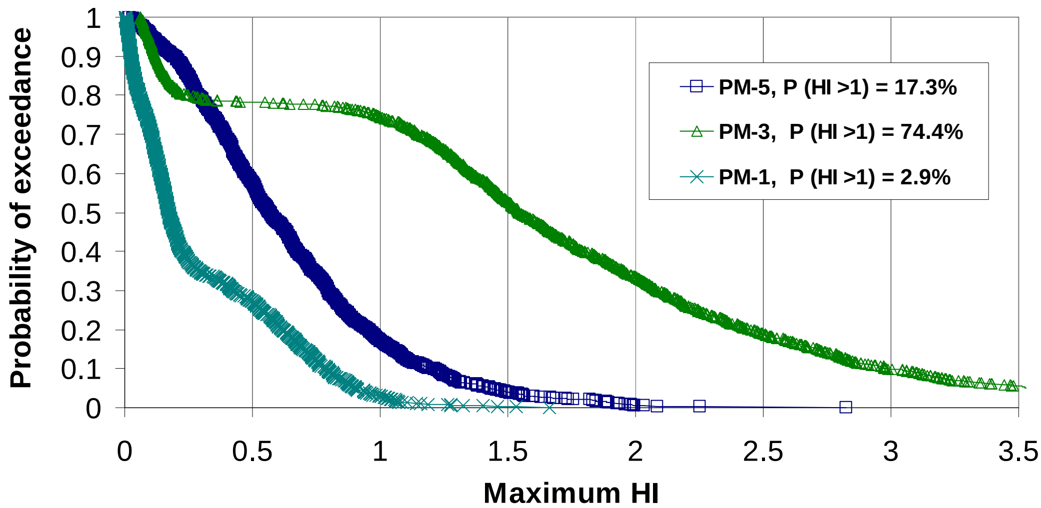

Fig. 1 Baseline risk assessment results shown as complementary cumulative distribution functions for one conceptual model. Numbers in the legend indicate the probability of exceeding an HI value of 1.0 for each of three production wells.

Designators PM 1, 3, and 5 in Fig. 1 refer to existing water supply wells. These are a subset of the wells analysed. Less than 5% of the simulated HI values for most of the wells exceed 1.0. In other words, the resulting risk is acceptable for most wells. Well PM-5 results indicate that 17.3% of the results exceed an HI of 1.0 while 74.4% of the PM-3 results exceed an HI of 1.0. Therefore, some risk-management activity is needed to avoid adverse human-health affects at PM-3 and PM-5. Other vadose-zone conceptual models analysed by Hollis *et al.* (2005) produced similar results while the one alternative conceptual model for the regional aquifer indicated acceptable risk at all production wells. The following sections describe the general process of evaluating one particular type of risk-reduction activity, that is, additional site characterization.

Identifying risk-reducing data collection activities

As defined by the LANL DSP, risk includes uncertainty in our knowledge about the geohydrological system. Therefore, reducing uncertainty in parameter values and/or assumptions has the potential to reduce the calculated risk. A large number of model parameters are employed in groundwater flow and transport modelling. Not all of these parameters have an equal effect on calculated risks. Rank correlation and regression analysis are employed to identify the handful of parameters that have the largest impact on model results. The subset of parameters identified by these analyses is used in the remaining steps of the LANL DSP.

Next, the required reduction in parameter uncertainty needed to yield acceptable risk results is quantified. In this case, acceptable risk is 95% confidence that the HI value will be less than 1.0. This uncertainty reduction analysis involves searching the existing combination of sampled parameter values and associated HI results for limits on parameter values that would result in an acceptable probability of exceedence. Shown in Table 1 are the results of the uncertainty reduction analysis for well PM-5.

For PM-5, a number of parameters and one combination of parameters (Table 1) were identified whereby specified reductions in their uncertainty could lead to an acceptable probability of exceedence (95% chance that the HI values will be less than 1.0). For PM-3, no amount of parameter uncertainty reduction yields acceptable probabilities of exceedence. In other words, there is no value in additional site characterization for PM-3 and a different type of risk-reduction activity must be employed (ex., remediation, stabilization, etc.).

Table 1 Results of uncertainty reduction analysis for PM-5.

Input variable parameter	Value in initial distribution	Value required to achieve 95% confidence
Maximum infiltration rate (m year^{-1})	4.471	1.061
Minimum porosity of the Santa Fe Fanglomerate	0.011	0.095
Maximum infiltration rate (m year^{-1}), and porosity of the Santa Fe Fanglomerate	4.471 0.011	1.25 0.0275

Comparison of risk-management alternatives

Risk management alternatives are presented in terms of expected cost and time to completion. Expected cost is the product of probability of success and likely cost. In the example risk-management activity described above, additional site characterization, the probability of success is the probability that given activity will yield the expected results. Taking one of the site characterization examples above—the porosity of the Santa Fe Fanglomerate—the probability of success is the probability that additional site characterization can prove that the minimum porosity is greater than 0.011. This probability is estimated by the same subject matter experts who aided in the definition of the original PDF for this parameter. Estimation of the probability of success forces the analyst to face the very difficult but important question of how future measurements can affect the current state of knowledge. Therefore, in addition to the number of measurements required to change the current state of knowledge, questions such as measurement location, scale and representativeness must be addressed. However, it is important to keep in mind that the estimated probability affects only the decision process. No change is made to actual risk assessment until measurements are performed, analysed, and incorporated into the parameter PDF.

In addition to potential site characterization activities, the general LANL DSP process involves estimating the same quantities (probability of success, cost, and time to completion) for all other available risk management activities, including, but not limited to, source control, remediation, land-use restriction, and/or monitoring. The LANL DSP does not take the final step of mathematically defining the "optimal" decision. Instead the attributes of all risk-management activities are provided to LANL management, the regulators, and the public in the recognition that factors outside of risk play an important role in the decision making process.

SUMMARY

LANL has developed a decision support process that: (1) seeks to *prioritize* risk management activities (e.g. characterization, stabilization, monitoring, remediation alternatives) *based on the risk* posed by the facility; (2) *quantitatively* integrates all knowledge related to risk (e.g. contaminant distribution, transport, fate, receptors, exposure); (3) provides a *quantitative assessment* of the value of alternative risk management actions (e.g. risk reduction per action, cost, etc.); and (4) for characterization, identifies additional data sufficient to reduce uncertainty *to the degree necessary to change a decision.*

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