Model-Assisted Decision Analyses Related to a Chromium Plume at Los Alamos National Laboratory – 15449

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ABSTRACT

The chromium plume at Los Alamos National Laboratory is a complex contaminant-remediation site with spatial extent of several square kilometers. It is located in a regional aquifer near water-supply wells and other points of compliance. The plume originated on the ground surface and the contaminant migrated along complex pathways through a thick vadose zone (~300m) that incudes intermediate lateral zones of saturation and vertical preferential flowpaths. Here we discuss the development of a modeling computational framework for the site. The framework work incorporates data assimilation and model-results analysis tools including decision support techniques. The decision tools are demonstrated using synthetic problems consistent with the interpretation of existing site data and site modeling results. The analyses aim at robust and efficient environmental management of the plume and explore a series of alternative remedial options. The remedial options include natural attenuation (NA), enhanced attenuation (EA), contaminant source removal (in the vadose zone), contaminant extraction (in the regional aquifer at the plume centroid and peripheries), biogeochemical remediation (injection of fluids stimulating growth of organisms in the aquifer impacting chromium concentrations), as wells as hydraulic controls on the groundwater flow and transport in the vadose zone and the regional aquifer. The applied model analyses and decision-support algorithms are implemented in code MADS (Model Analyses for Decision Support; http://mads.lanl.gov). MADS is an open-source framework for model-based decision support employing system and physics simulation models.

INTRODUCTION

There is a pressing need for better tools that empower remedy selection for contaminated groundwater. The U.S. National Research Council recently estimated that the cost to clean up (i.e., remediate) sites that federal law mandates be remediated is over $100 billion with the Department of Energy's burden being approximately $20 billion [1]. Uncertainty plagues remedy selection. There is often substantial uncertainty in the contamination extent and concentrations, the rate and location at which contamination reaches the aquifer, the rate at which biogeochemical reactions are attenuating or exacerbating the problem, the direction and velocity of the groundwater flow, the rate and type of dispersion, diffusion and pore-scale mixing, large- and small-scale geological features and heterogeneities as well as performance and effectiveness of remedial actions; this list includes parametric and conceptual (potentially “deep”) uncertainties. The list could go on and each of these uncertainties could be further subdivided and expanded. On top of the listed known-unknowns, there are also unknown-unknowns. The unknown-unknowns are uncertainties for which we are currently unaware but potentially can have important impact on the decision processes. It is therefore not surprising that according to U.S. National Research Council report, court mandated remediations fail almost 90% of the time, often due to unforeseen uncertainties and complexities [1].

Decision-making process for environmental management of contaminated sites includes the development and selection of remediation strategies. Scientifically defensible evaluation of specific remedial actions in terms of both their environmental benefits and cost effectiveness requires a robust conceptual model of

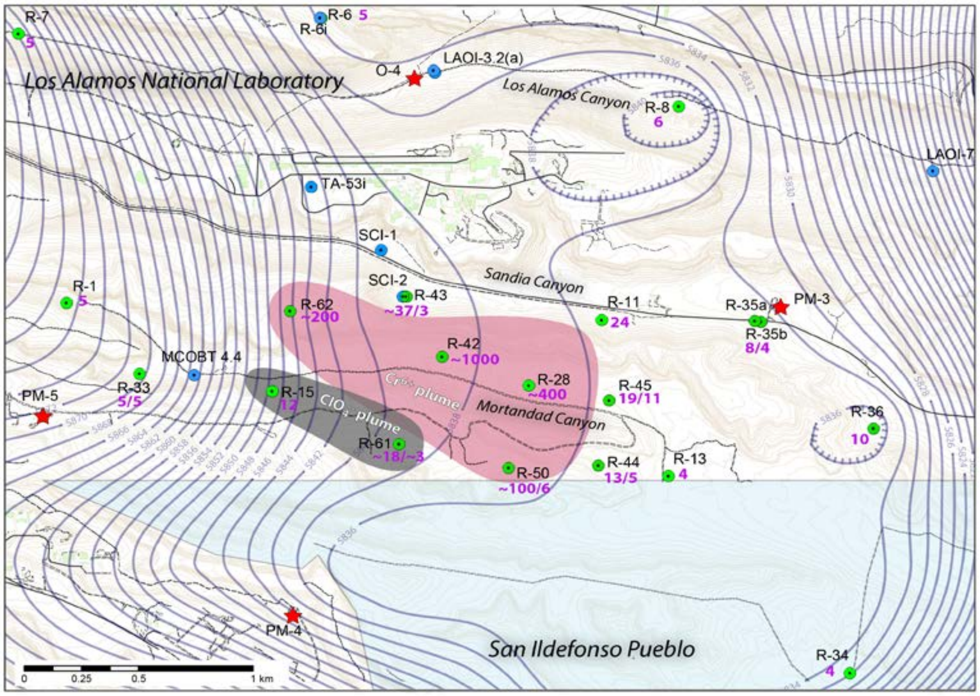

Fig. 1: Location of the study site. Green and blue dots show the locations of aquifer and vadose zone monitoring wells, respectively. Red stars are municipal water supply wells. Recently observed Cr^{6+} concentrations (circa 2014) at each regional well are shown in purple [μg/ℓ]; the concentrations at two-screen wells (e.g. R-61) are shown as upper / lower screen values. The Cr^{6+} plume represents an area where concentrations are higher than 50 μg/ℓ (ppb).

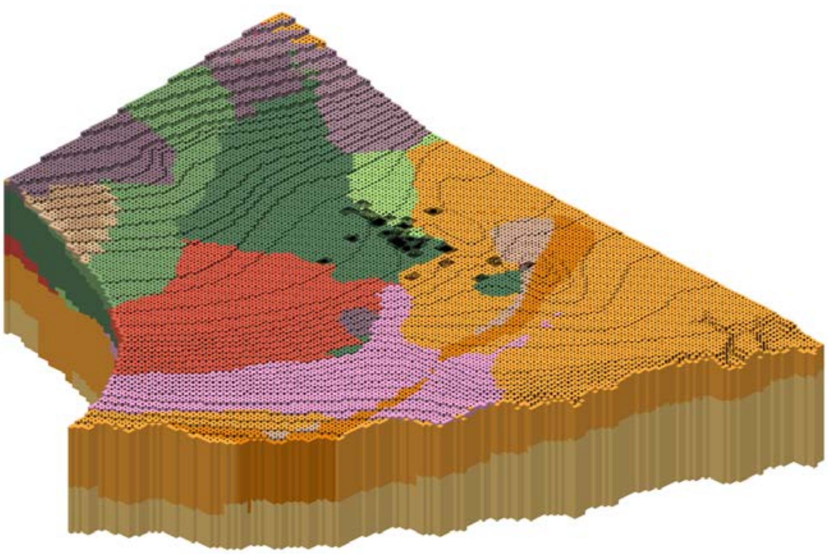

Fig. 2: Computational grid. The black regions on the top of the model grid define the well locations. The colors represent hydrostratigraphic. The top of the model represents the regional water table. The front side boundary is aligned along Rio Grande.

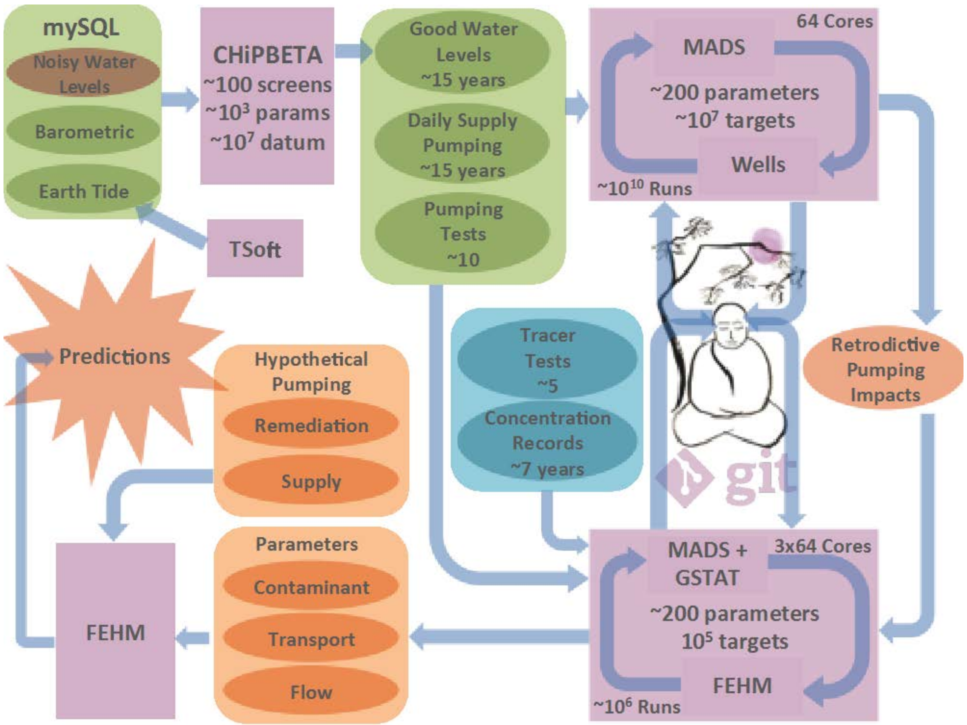

Fig. 3: Modeling workflow.

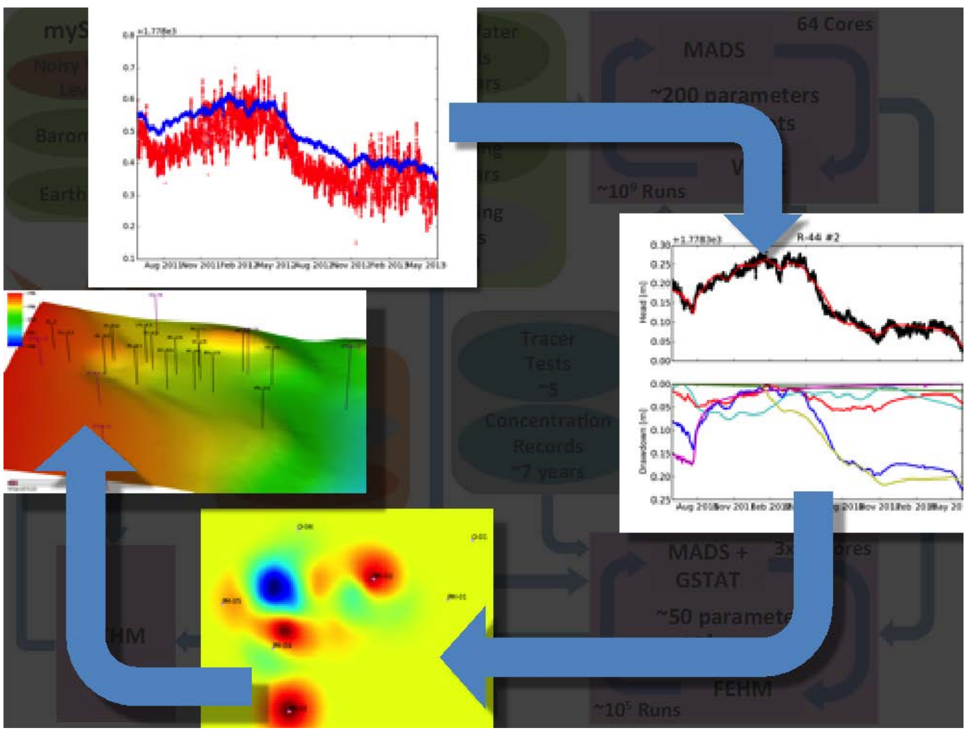

Fig. 4: Modeling workflow: from observed data (a) to model-estimated drawdowns (b), to model-estimated aquifer heterogeneity (c) to model-predicted groundwater flow directions (d).

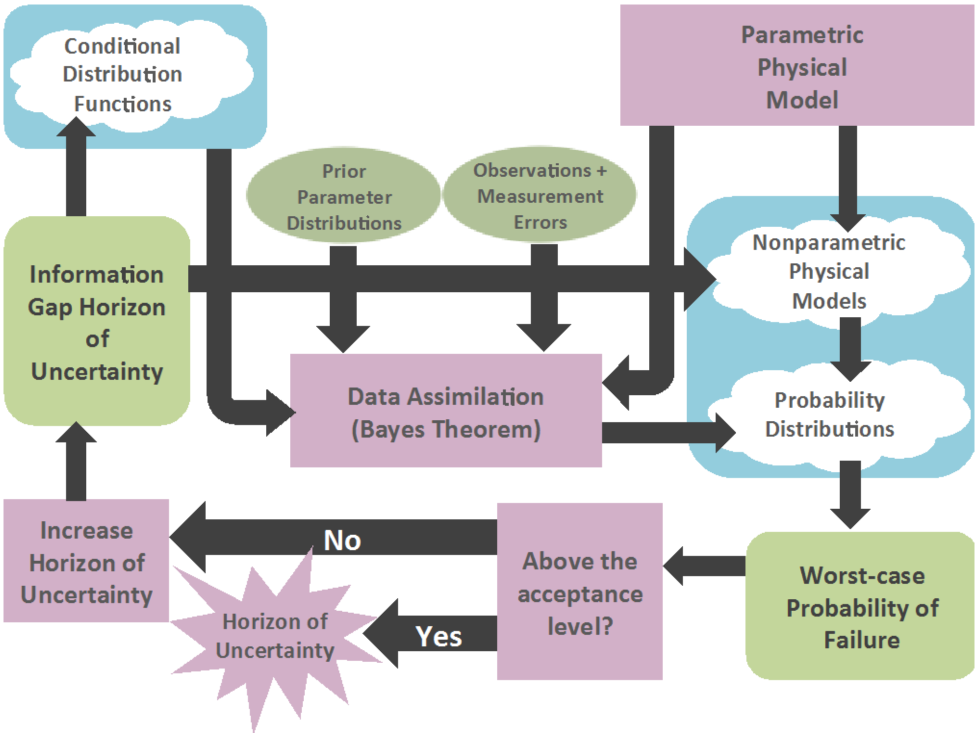

Fig. 5: Bayesian Information Gap (BIG) decision analysis.

the site and systematic characterization of conceptual model elements related to processes governing contaminant migration in the subsurface. Conceptual model uncertainties can be estimated based on detailed analyses of the available qualitative and quantitative site knowledge. The decision process also identifies potential data and conceptual-understanding gaps requiring additional data acquisition to refine remedy selection. The decision-making process is facilitated by implementation of robust computational techniques for decision support that take into account existing site uncertainties. However, due to data and knowledge gaps as well as complex interdependencies between uncertainties (conceptual elements, model parameters, measurement/computational errors, etc.), the decision-support optimization problem is typically non-unique, and the model-prediction uncertainties are frequently difficult to quantify. The problem is non-unique because multiple solutions produce reasonable agreement with the site data. [2-4]. We have performed detailed investigation of site information related to a chromium plume in groundwater beneath Los Alamos National Laboratory (LANL). Over the years, we have performed detailed investigations of the site information including hydrogeological, geophysical, petrographic, and geochemical studies for site characterization. We have also developed a series of alternative conceptual and numerical models representing governing subsurface processes with different complexity and at different scales (resolutions). The current site conceptual model is supported by multiple lines of evidence from alternative analyses of the available data [5-8].

A map of the LANL contamination related to a chromium (Cr^{6+}) plume in the regional aquifer beneath Sandia and Mortandad Canyons is presented in Fig. 1 [9]. The site computational grid and the model domain for one of the three-dimensional numerical models developed for the site is presented in Fig. 2 (for more information see [10]). The modeling workflow incorporates numerous computational tools and data streams presented in Fig. 3. In the context of these modeling workflow, a conceptual representation of how data are assimilated to produce model predictions of water-level drawdowns, aquifer heterogeneity and groundwater flow is presented in Fig. 4. The developed modeling workflow is embedded in a decision framework presented in Fig. 5. The decision framework is described in the next section.

METHODOLOGY

The goal of the decision analyses is to provide scientifically defensible and economically feasible solutions to a complex contaminant remediation problem. The evaluation of remedial actions is based on their anticipated environmental impact. The conceptual model uncertainties are estimated based on detailed analyses of the available qualitative and quantitative site data. The decision process also identifies data and conceptual-knowledge gaps requiring additional data acquisition to refine remedy selection. The decision-making process is facilitated by implementation of robust computational techniques for decision support taking into account all the existing site uncertainties.

Bayes' theorem is one of the most popular techniques for probabilistic uncertainty quantification (UQ). It is effective in many engineering situations, because it updates our understanding of the uncertainties by conditioning on real data using a mathematically rigorous technique. Bayes' theorem is mathematically rigorous, but its application in science and engineering is not always rigorous. There are **two issues** associated with practical application of Bayes' theorem.

Issue 1: We can enumerate the possible outcomes of dice rolling, but not the possible outcomes of groundwater contamination remediation. For example, we cannot enumerate all the possible permeability fields that we can expect at a given site. Similarly we cannot enumerate all the possible outcomes of remedial activities.

Issue 2: We can precisely determine conditional probabilities for coin tossing, but substantial uncertainty surrounds the conditional probabilities for groundwater contamination remediation. For example, we may have a given field observation (e.g. concentration of 50 ppb at a given monitoring well) and we may have a series of models that predict concentrations close to the observed value (e.g. model A and B predict 51 and 49 ppb, respectively); in this case, it is challenging to define the likelihoods (conditional probabilities) of the models given this concentration information.

Bayes' theorem is rigorously applicable beyond dice rolling and coin tossing, but applying Bayes' theorem to the real world may not work as well as one might expect. Bayes' theorem is rigorously applicable only if all possible events can be described, and their conditional probabilities can be derived rigorously. To overcome these issues, we employ a Bayesian Information Gap Decision Analysis. Bayes' theorem is applied for conditioning on available data, capturing the parametric uncertainty. The methodology employs a non-probabilistic uncertainty quantification (UQ) methodology called Information-Gap Decision Theory (IGDT) to capture conceptual model uncertainty (overcoming ***Issue 1*** above) and uncertainty in the conditional probabilities used in the application of Bayes' theorem uncertainty (overcoming ***Issue 2*** above). The decision workflow in conceptualized in Fig. 5. More details about the developed methodology are presented in [11]. Additional applications of Information Gap Decision Theory for groundwater problems are presented in [12-13]

The Bayesian-Information-Gap approach to UQ is independent of the physical model and implemented in the existing open-source MADS code [14-16]. This makes it possible to employ the approach on a laptop with simple physical models or a supercomputer with complex physical models. MADS is capable to perform various types of model analyses including sensitivity analysis, parameter estimation, uncertainty quantification, model calibration, selection and averaging. MADS is designed to provide an interactive computer-based Decision Support System (DSS) that will help domain scientist, managers, regulators, and stakeholders to make decisions related to site characterization, monitoring design, and remedial activities based on data- and model-driven decision-support analyses exploiting high-performance computing.

APPLICATION

The site conceptual model describes the processes controlling the movement of groundwater and contaminants in the environment. The current conceptual model is explained in detail in [8], and supported by multiples lines of evidence. The establishment of the current conceptual model involved field, laboratory and modeling analyses [8]. Based on the site conceptual model we developed two synthetic contaminant remediation problems. Additional information about the site conditions is presented in [17-18].

In the first scenario, a contaminant is released for one year (from t=0 to t=1 years; Fig.6). The contaminant is monitored at 19 wells as times ranging from 0 to 10 years. Data for the contaminant concentrations at the monitoring wells are synthetic and were produced via a computer simulation. The observations for the contaminant concentrations at the monitoring wells are computed assuming that the contaminant source is box-shaped with a constant mass flux and the plume undergoes advection with a constant drift, classical dispersion in the y and z directions, fractional Brownian dispersion in the x direction, and first-order decay (representative of in-situ contaminant degradation; for example, biogeochemical reduction). Of course, in practice, the contaminant concentrations at the monitoring wells will come from measurements rather than simulations. At t=10 years, a decision must be made concerning the remediation of the contaminant. The desired outcome is that the contaminant concentration at a point of compliance be below the MCL for the next 40 years (from t=10 to t=50 years. The source has dimensions 250 m x 250 m x 1 m. Two remedial actions are analyzed. One is the NA case, where it is deemed that naturally occurring biogeochemical reactions and dispersion are sufficient to reduce the contaminant concentrations below the Maximum Concentration Limit (MCL). The other is an approach to EA where a stimulant that converts the contaminant into an innocuous substance is injected into the contaminant plume (e.g., bioremediation induced by injection of oxidization agent such as alcohol). In the case of NA and EA, first order reactions are assumed. Parametric uncertainty is considered in the naturally occurring reaction rate and the mechanism of longitudinal aquifer dispersion.

In summary, there are 10 contaminant concentrations observed at each of 19 monitoring wells representing 190 data records. There are 2 uncertain model parameters with distributions informed via Bayes' theorem by the observed concentration data. The decision analysis proceeds by computing the decision robustness. Conceptually, this can be understood to consist of three nested loops. The outer loop iterates over increasing values of the horizon of uncertainty related to our information-gap decision model. The middle loop iterates over possible conditional distributions for the model parameters. The inner loop performs a Markov chain Monte Carlo iteration to sample from the posterior distribution for the model parameters. The samples are used to compute the probability of failure given the model uncertainty.

The decision-analyses results suggest that for both the NA and EA scenarios, the nominal probability of failure is approximately zero. Therefore a classical Bayesian analysis will predict that both remedial actions are equally good and there are no preference for performing EA over NA. However, this decision has zero robustness. Fig. 7 depicts the robustness (horizontal) versus acceptable probability of failure. The overall robustness of the two remediation approaches is found by locating the value of robustness where the curves intersect the dashed line in Fig. 7 which defines the maximal acceptable probability of failure. The decision robustness for the NA and EA scenarios are 0.34 and 0.78 respectively. This indicates that

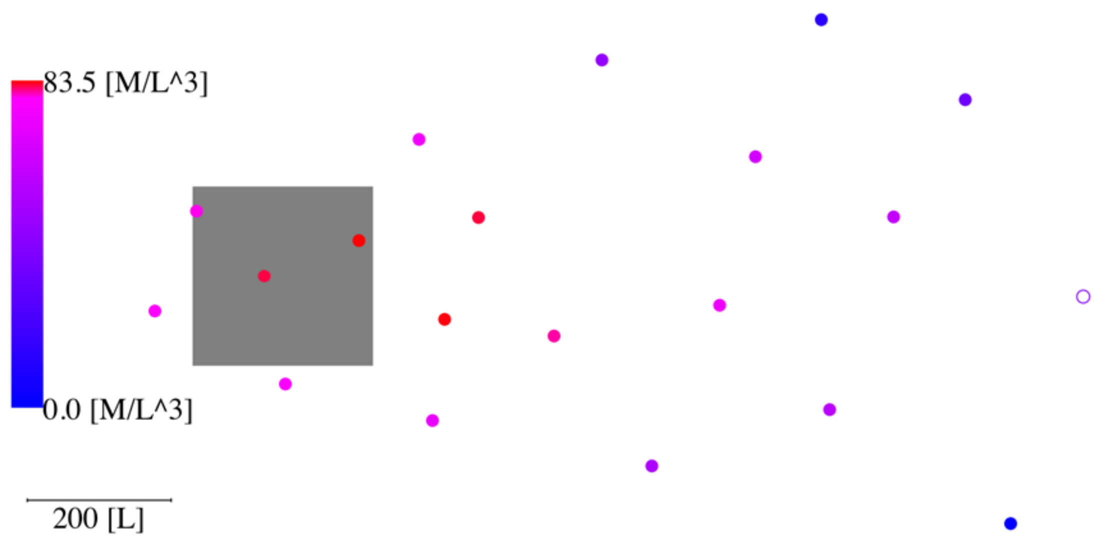

Fig. 6: Network of wells and contaminant source for scenario 1. The 19 monitoring wells are shown with filled-in circles, the contaminant source location is represented with a square, and the point of compliance is shown by a hollow circle. The colors show the observed concentrations at t=10 years.

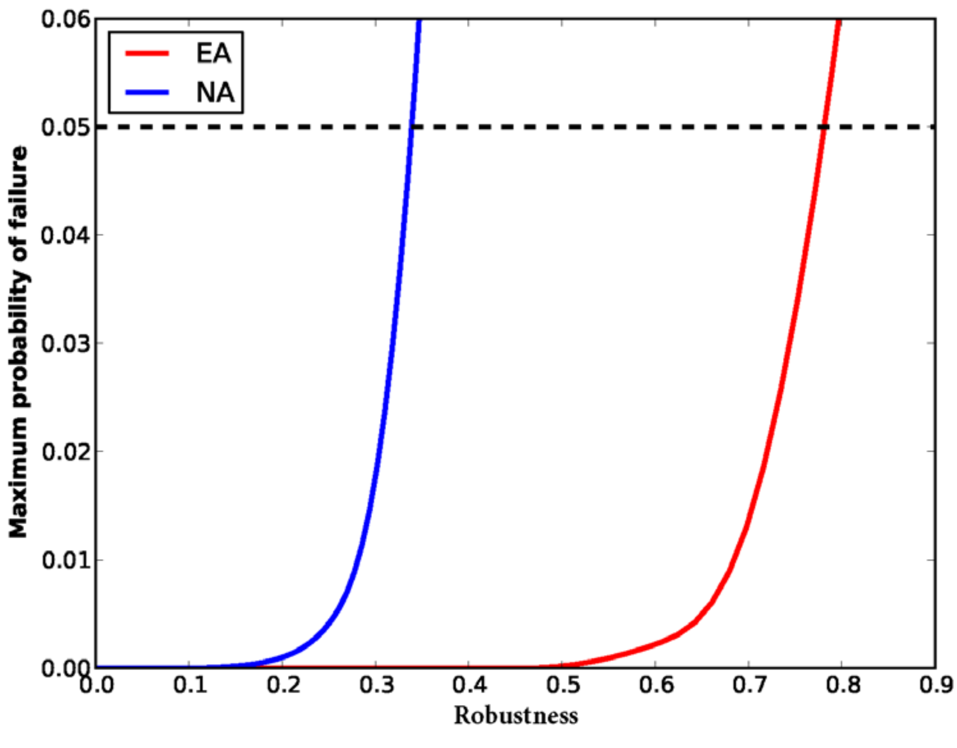

Fig. 7: The decision robustness (horizontally) as a function of the maximum chance of failure (vertically) for scenario 1. With both remediation approaches, the nominal chance of failure is approximately zero when the robustness is equal to zero. However, the maximum chance of failure remains low over a substantially larger uncertainty range for EA compared to NA.

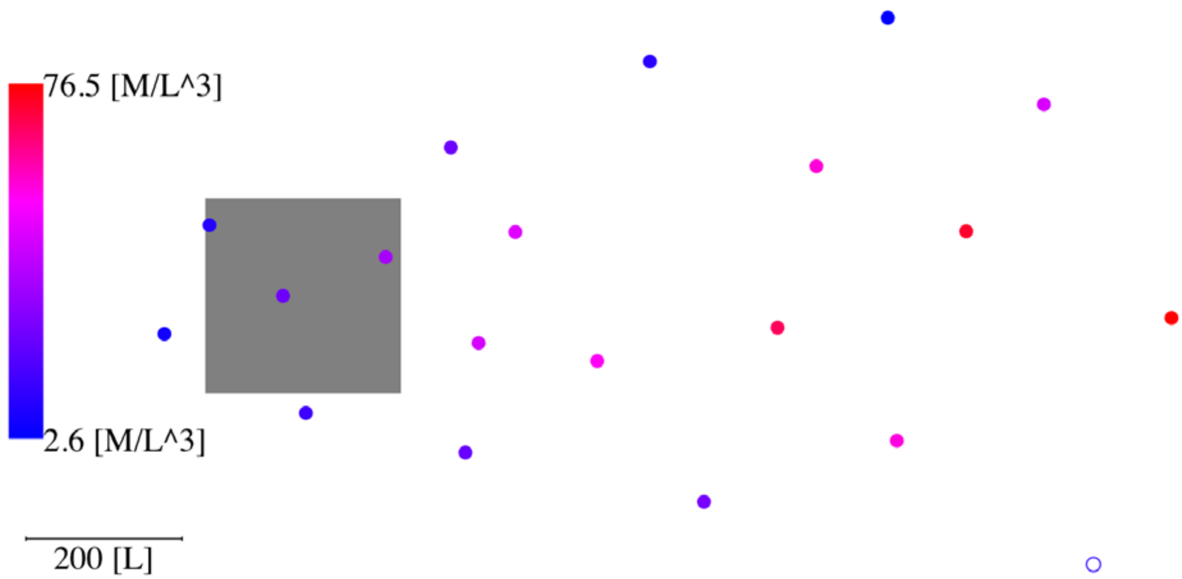

Fig. 8: Network of wells and contaminant source for scenario 2. The 19 monitoring wells are shown with filled-in circles, the contaminant source location is represented with a square, and the point of compliance is shown by a hollow circle. The colors show the observed concentrations at t=10 years.

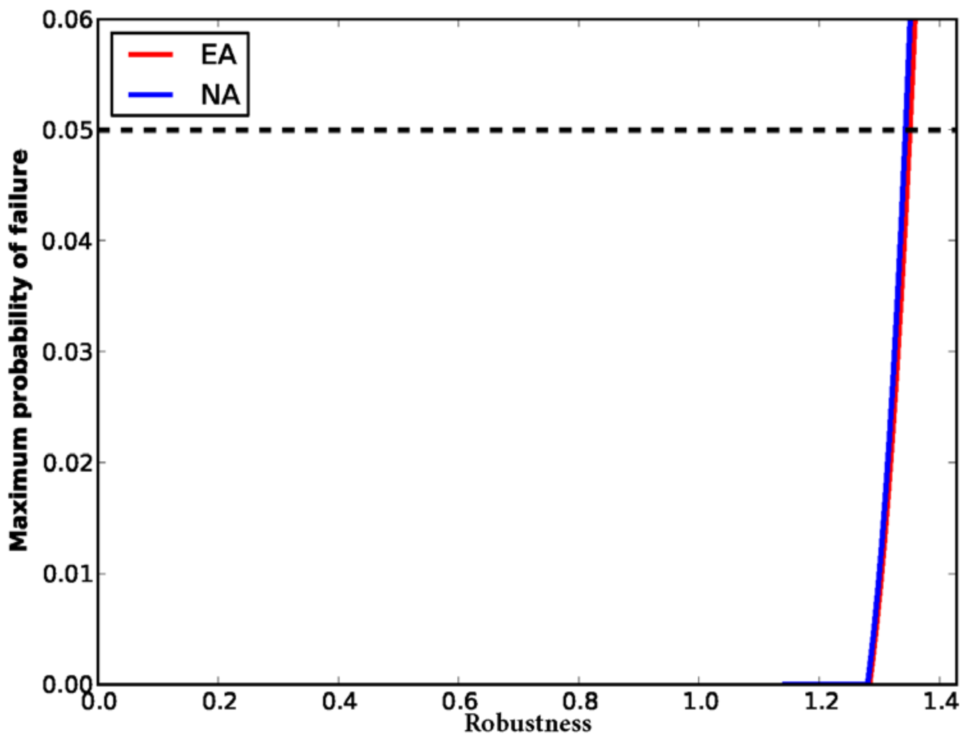

Fig. 9: The robustness (horizontally) as a function of the maximum chance of failure (vertically) for scenario 2. Note that in this scenario, the EA approach provides little additional robustness.

substantially more uncertainty can be tolerated by EA before the failure might be possible. The robustness value of 0.34 for NA means that the concentrations may exceed the MCL with only a 34% model error and within a relatively small window around the nominal conditional distributions. Relative to the severe uncertainties typically present in subsurface remediation problems, this is a modest amount of uncertainty. Therefore, and despite the fact that the nominal probability of failure for NA is nearly zero, it would be prudent in this scenario to perform the EA remediation strategy. The maximum probability of EA failure increases rapidly providing further support for this perspective.

In the second scenario, the location of the compliance point is modified (Fig. 8). The compliance point has been relocated and it is not aligned with the transport direction of the contaminant plume center of mass. Fig. 9 plots the robustness (horizontally) as a function of the maximum chance of failure (vertically). In this scenario, both remediation approaches have a small chance of failure over a relatively large uncertainty ranges. The robustness for the EA approach is approximately 1.35, compared to 1.34 for the NA approach. In this scenario, the NA approach is likely to succeed even after allowing for substantial modeling error (134% model error) as well as a relatively broad neighborhood around the nominal conditional distribution used in Bayes' theorem. Therefore, the NA approach may be sufficient in this case. The EA approach provides only a very small amount of additional robustness. Therefore, it is not a strong alternative to the NA approach. If the robustness provided by NA is insufficient, the robustness provided by EA is very likely to be insufficient as well. In this case, it may be prudent to find an alternative remediation approach which can be also included in the presented decision support framework. In this scenario, the decision analyses suggest that the EA does not substantially increase the robustness. By the time the EA has been implemented, the peak concentrations have already been observed at the compliance point. The aquifer dispersion has a much stronger impact on reducing the contaminant concentrations at the point of compliance than increasing the reaction rate. In this scenario, it would not be practical to perform the EA. If the robustness provided by NA is deemed insufficient, and alternative remediation approach should be pursued.

CONCLUSIONS

Unknowns and uncertainty play a significant role in selecting a remedy for contaminated groundwater. Measurement errors, parametric uncertainties, and model inadequacies all contribute to these unknowns and uncertainties. We have described a decision support framework that takes these unknowns and uncertainties into consideration. The framework represents a general, comprehensive, and novel approach for dealing with a diverse range of uncertainties and unknowns associated with model-based decision analyses. Applications of this approach are not limited to groundwater remediation problems. It can applied to engineering fields that combine data and models to make decisions: *e.g.*, climate change, energy production, waste storage, carbon sequestration, *etc*.

All the applied computational tools are embedded in the code MADS (http://mads.lanl.gov), which provides a computationally efficient and robust framework for various types of model analyses related to decision support; it also includes advanced novel optimization techniques [e.g. 19-20]. This allows for computationally efficient, reproducible and defensible model-based analyses for decision support. Currently, MADS algorithms are also being implemented in a Decision Support Toolbox of ASCEM (*Advanced Subsurface Computing for Environmental Management*; http://ascemdoe.org) code development project funded by the U.S. *Department of Energy, Environmental Management*. ASCEM targets development of an interactive computer-based Decision Support System (DSS) that will help domain scientists, managers, regulators, and stakeholders make decisions related to site characterization, monitoring design, and remedial activities based on data- and model-driven decision-support analyses exploiting high-performance computing [21-22].

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