Decision Analyses Related to Groundwater Remediation – 17051

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ABSTRACT
Traditional decision analyses of groundwater remediation scenarios frequently fail because the probability of adverse, unanticipated events occurring is often high. This is driven by many factors including that (1) the models developed to represent the flow and transport in contaminated aquifers are typically simpler than reality and do not account for all the important governing processes, (2) probability distributions are assigned to critical performance parameters (such as model inputs or characteristics of the engineered remediation systems) even though some of these parameters might be unknown or not be very well constrained. However, there is a novel decision analysis methodology and a computational tool based on Bayesian Information-Gap Decision Theory (BIG-DT) that are designed to mitigate the shortcomings of the models and probabilistic decision analyses by leveraging a non-probabilistic decision theory -- information-gap decision theory. The new decision analysis methodology considers possible models that have not been explicitly enumerated and does not require us to commit to a particular probability distribution for model and remediation-design parameters. Both the set of possible models and the set of possible probability distributions grow as the degree of uncertainty increases. The fundamental question that BIG-DT asks is “How large can these sets be before a particular decision results in an undesirable outcome?”. The decision that allows these sets to be the largest is considered to be the best option. In this way, BIG-DT enables robust decision-support for groundwater remediation problems. Here, we apply BIG-DT to a representative groundwater remediation scenario where different options for hydraulic containment and pump & treat are being considered. BIG-DT requires many model runs and high-performance computing resources are needed when complex models are used. We demonstrate the BIG-DT analyses on a series of synthetic problems that are designed to be consistent with real-world problems such as Los Alamos National Laboratory (LANL) contamination sites. We also discuss a general framework for how the BIG-DT analyses will be carried out at the chromium groundwater contamination site at LANL. BIG-DT is implemented in Julia (a high-level, high-performance dynamic programming language for technical computing) and is part of the MADS framework (http://mads.lanl.gov and http://madsjulia.github.io/Mads.jl).

INTRODUCTION
Recently, O'Malley and Vesselinov [1] presented a Bayesian-Information-Gap Decision Theory (BIG-DT) framework for making decisions under various types and severities of uncertainty. O'Malley and Vesselinov [2] applied BIG-DT to site selection for CO_2 sequestration. In the current work, we demonstrate the application of BIG DT for groundwater remediation. BIG-DT analysis is performed using the open-source code MADS (Model-Analyses & Decision Support) [3,4]. The analyses are based on synthetic example problems. However, they are designed to be consistent and representative of the conditions at the Los Alamos National

Laboratory (LANL) Chromium site [3].

LANL CHROMIUM SITE

The chromium plume at LANL 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. The remedial options at the site 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. For the last 7-10 years, a substantial amount of research and model-analysis work have been actively applied at the site [5–7]. A site map is presented in Fig.1. The figure shows the locations of the site monitoring wells and observed chromium concentrations.

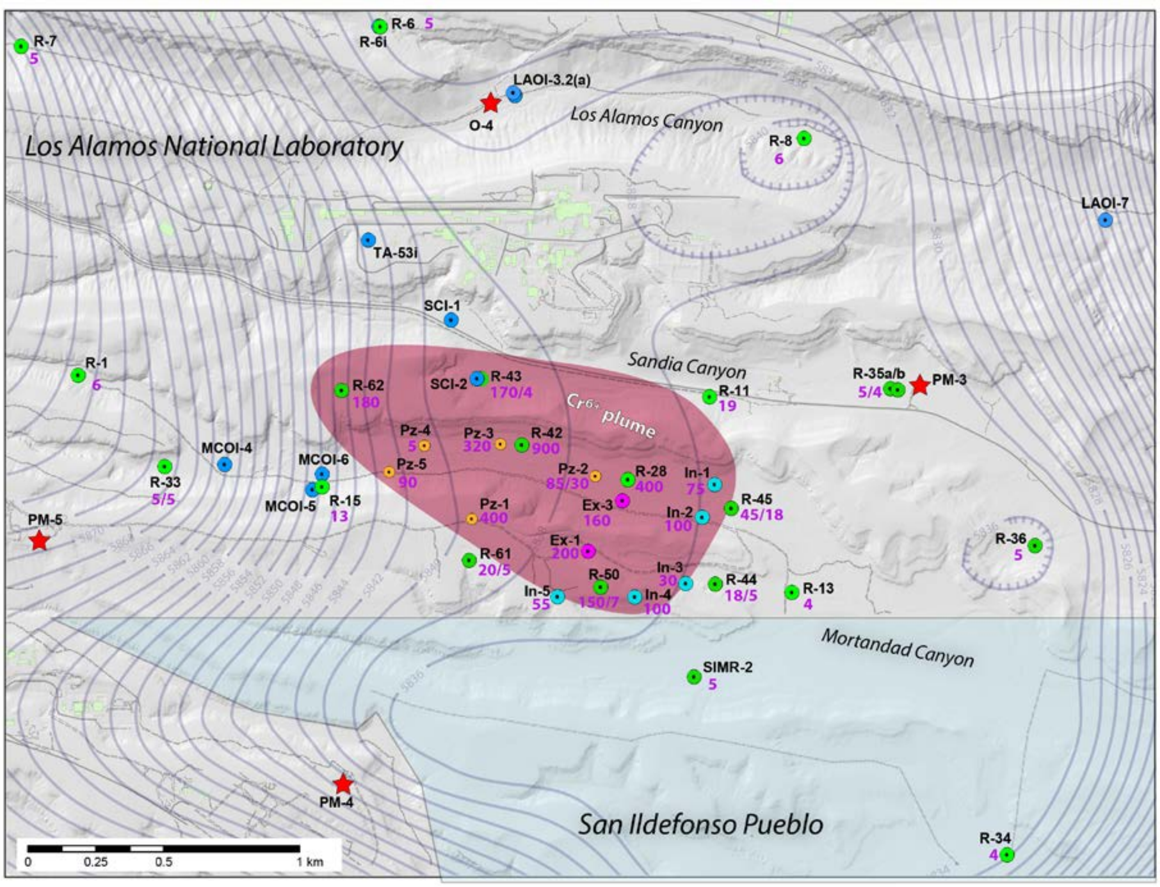

Fig. 1: Map of the LANL chromium site representing site conditions circa 2016. Green and blue dots show the locations of aquifer and vadose zone monitoring wells, respectively. Red stars are municipal water supply wells. Recently observed chromium (Cr^{6+}) concentrations at each regional well are shown in purple [μg/ℓ]; the concentrations at two-screen wells (e.g. R-61) are shown as upper / lower screen

values. The chromium plume (red) represents an area with concentrations higher than 50 μg/ℓ (ppb).

BIG-DT METHDOLOGY

BIG-DT is a novel approach that uses a combination of site observations, modeling, Information Gap Decision Theory (IGDT), and Bayesian statistics to perform model-based decision analyses. The framework allows decision makers and stakeholders to make a decision under various types and severities of uncertainty in a rigorous and mathematically justifiable manner.

Bayes' rule is a commonly used tool for inverting probabilities. In the case of non-deterministic (probabilistic) models, there are uncertain model-input parameters that produce uncertain model-predicted outcomes. The uncertain inputs and outputs are often defined by a probability distribution function (*pdf*). Bayes' rule allows us to estimate probability of input parameters given probability of the outcomes. In other words, Bayes' rule allows us to use measured uncertain site observations related to the corresponding model outputs (predictions), to make an inference about the input model parameters. Bayes' rule can be defined mathematically as,

$$f(\mathbf{q}|\mathbf{o}) = \frac{f(\mathbf{q}|\mathbf{o})\ f(\mathbf{q})}{\int_{\Omega} f(\mathbf{q}|\mathbf{o})\ f(\mathbf{q})\ d(\mathbf{q})} \quad (1)$$

where $\mathbf{q}$ are the model-input parameters, Ω is the model-input parameter space, $\mathbf{o}$ are observations, $f(\mathbf{q})$ is the prior distribution, and $f(\mathbf{q}|\mathbf{o})$ is the likelihood function. The prior distribution represents our belief about how the parameters of the system are distributed *a priori* (based on literature data or expert knowledge). The conditional likelihood function is a function that describes how the observations are distributed given model-input parameters $\mathbf{q}$. The conditional likelihood function is generally related to the discrepancies (residuals) between observed data and model predictions (model output for given $\mathbf{q}$) [8].

In practice, the integral in the Bayes' rule equation is difficult to compute analytically because the exact form of the model function is typically complex and unknown; the model function is frequently high dimensional over the entire model-input parameter space. Monte Carlo methods are frequently used instead to approximate a solution to the Bayes' rule equation. In the BIG-DT approach, Bayes' rule is used to address parameter uncertainty.

Information-Gap Decision Theory (IGDT) (also referred as Info-gap Decision Theory) is a non-probabilistic method for quantifying uncertainty. IGDT answers the following question: “How wrong can our best guess be before the possibility for failure exists?” IGDT does not consider the probability of events to occur, but instead it focuses only on exploring sets of events that are important for the decision analysis [9]. IGDT application is motivated because the classical (Bayesian) probabilistic methods fail to adequately characterize uncertainties in the following cases:

- <u>Uncertainty cannot be characterized by assigning a probability to all possible events</u>. For example in many real-world remediation problems, there are multiple different conceptual models that can be applied to represent physical processes at a site. As a result, frequently, it is impossible to define all possible conceptual models, and it is impossible to the define the probability for each conceptual model to occur.

- The actual probability distribution function (*pdf*) that characterizes the uncertainty is unknown. In many real-world problems, we know there are uncertainties, but we do not know what is the type (shape) of the *pdf* describing each uncertainty. We do not know if they are uniform, normal, log-normal, Levy type, or something else; typically we do not even know basic properties of the *pdf* (mean, variance, etc.). In this case, guessing the *pdf* type/ properties, even if it is approximately correct causes a bias. The guessed *pdf* model is imposing information into the decision process that is quite possibly untrue. For example, major consequences can occur from performing decision analyses at the tails of the guessed *pdf* that may differ substantially from that of the actual unknown *pdf* [10]. Frequently events in the tails of the distribution are exactly what decision makers are interested in, because these events typically represent extreme events, and therefore may be a disaster that a decision maker is trying to avoid.

Mathematically, the info-gap model can be expressed as,

$$M(\varepsilon, \mathbf{q}) = \left\{ F : \left| \frac{F_i - F_i(\mathbf{q})}{F_i(\mathbf{q})} \right| \leq \varepsilon, i = 1, 2, \ldots, N \right\} \tag{2}$$

where $M(\varepsilon, \mathbf{q})$ represents a set of possible outcomes from given set of parameters $\mathbf{q}$, within a horizon of information-gap uncertainty ε. We note that we have represented the model uncertainty here non-parametrically. This is important, because studies have shown that non-parametric model uncertainty can be significantly larger than parametric uncertainty [11]. The outcomes $M(\varepsilon, \mathbf{q})$ are all possible model outputs (predictions) that lie within a relative error of the nominal model $F_i(\mathbf{q})$, or expressed differently, all possible model outputs for which the relative maximum difference (infinity norm) between the possible model output and nominal model output, is less than or equal to a chosen horizon of uncertainty. The nominal model ($F_i(\mathbf{q})$) is the term used to identify the best guess for a particular phenomenon.

Note that, at a horizon of uncertainty of zero, BIG-DT analysis will be equivalent to a purely Bayesian analysis. Since the aim of IGDT is to answer the question: “How wrong can our best guess be before the possibility for failure exists?”, in terms of the info-gap model defined in Equation 2, this question can be answered mathematically as the largest set of possible outcomes for which none of the outcomes within the set causes failure as defined by the performance goals in the BIG-DT analysis. The largest horizon of uncertainty for which failure is not in the set of possibilities will be defined as the robustness of the decision [10]. IGDT allows one to quantify how robust a decision is against failure.

In order to calculate robustness in the BIG-DT analysis, one must first define what constitutes a failure. The criteria that define whether or not a failure has occurred will be referred to as performance goals. These are criteria that a decision maker would attempt to meet when choosing remedial options:

- Choose a remediation scenario that successfully remediates the groundwater.
- Choose a remediation scenario that avoids adverse affects to the aquifer.

With these criteria in mind, two performance goals that have been used in the current work to define failure, and are expressed mathematically as:

- The maximum concentration at a point of compliance does not exceed the MCL.
- The drawdown at water supply wells that is induced by the pump and treat system does not exceed a prescribed threshold.

BIG-DT is the confluence of two methods -- Bayesian and IGDT -- for addressing uncertainty with the aim of combining the strengths of each. Bayesian statistics are used to address the parametric uncertainty of the physical system. If the probability distribution of the observation errors was known and the physical model was perfectly accurate, the Bayesian approach would suffice at addressing all potential uncertainties. However, this is not the case. IGDT is used to address uncertainty that the Bayesian approach is not always well suited to address, namely: uncertainty in the physical model and uncertainty in the conditional likelihood function for the Bayesian approach (which describes the inaccuracy of the model and the observations). Uncertainty in the conditional likelihood is expressed as

$$U(\varepsilon) = \left\{ f_H(\mathbf{O}|\mathbf{q}) \colon \left|\frac{H-H_0}{H_0}\right| \leq \varepsilon, H \in [0.2, 0.8] \right\} \quad (3)$$

where $H_0 = \frac{1}{2}$ and $f_H(\mathbf{O}|\mathbf{q})$ is a multivariate Gaussian likelihood with covariance given in Equation 1 and zero mean. Note that in another study, a different info-gap model of the conditional likelihood could be used capture uncertainty in this function. Here, we have used the parameter H to describe uncertainty in conditional likelihood. In the info-gap uncertainty models (Equations 2 and 3), the index ε is used to describe a set of events that are possible within that horizon of uncertainty.

RESULTS

BIG-DT provides a unique capability for groundwater remediation, a ~$20 billion problem within the DOE complex [1]. We demonstrate this method by applying it to a problem that is representative of LANL's chromium plume. Fig.2 shows a schematic description of the representative site that we consider here. The commonalities with LANL's chromium site include: a network of ~30 monitoring wells surrounding the contaminant plume, a compliance boundary where concentrations must be kept below a regulator-specified threshold, supply wells in the vicinity of the contaminant plume, one or more wells that can be used for pump & treat near the boundary, and uncertain model parameters that govern the flow of water and transport of the contaminant. In this problem, three potential remedial options are considered. The first is the most expensive and involves using all three extraction wells. The second is the least expensive and involves only using the central extraction well. The third comes with an expense somewhere between the first two options and involves using the two outer extraction wells, but not the central extraction well.

Fig. 3 shows the results of applying BIG-DT to this decision scenario. As expected, the first remedial option provides the most robustness against uncertainty. Initially, it may be somewhat surprising that the second option (where only the central extraction well is used) provides more robustness against uncertainty than the third option (where the two outer extraction wells are used). However, this can be understood to arise from the fact that the central well is the crucial well for successful pump & treat here. When only the two outer wells are used, the contaminant can split the two wells make it across the compliance boundary.

CONCLUSIONS

Based on the presented BIG-DT analysis, we draw the following conclusions:

1. The least expensive remedy (use only the central extraction well) provides almost as much robustness against uncertainty as the best remedy (use all the extraction wells), making it a good option. The decision to use all the extraction wells could be justified if additional robustness is desired, and could be seen as a conservative decision.
2. Using the two outer extraction wells without using the central extraction well is not a good remedy, and employing this remedy would be a bad decision. It is expected to fail, and provides no robustness against uncertainty. If a two-well remedy is desired an alternative design should be considered such as employing the central well and one of the outer wells.

Currently, we are working on BIG-DT analyses related to actual real-world problems. More examples of synthetic application related to IGDT and BIG-DT can be found at http://madsjulia.github.io/Mads.jl/Examples/. For more information about MADS, please visit http://mads.lanl.gov/.

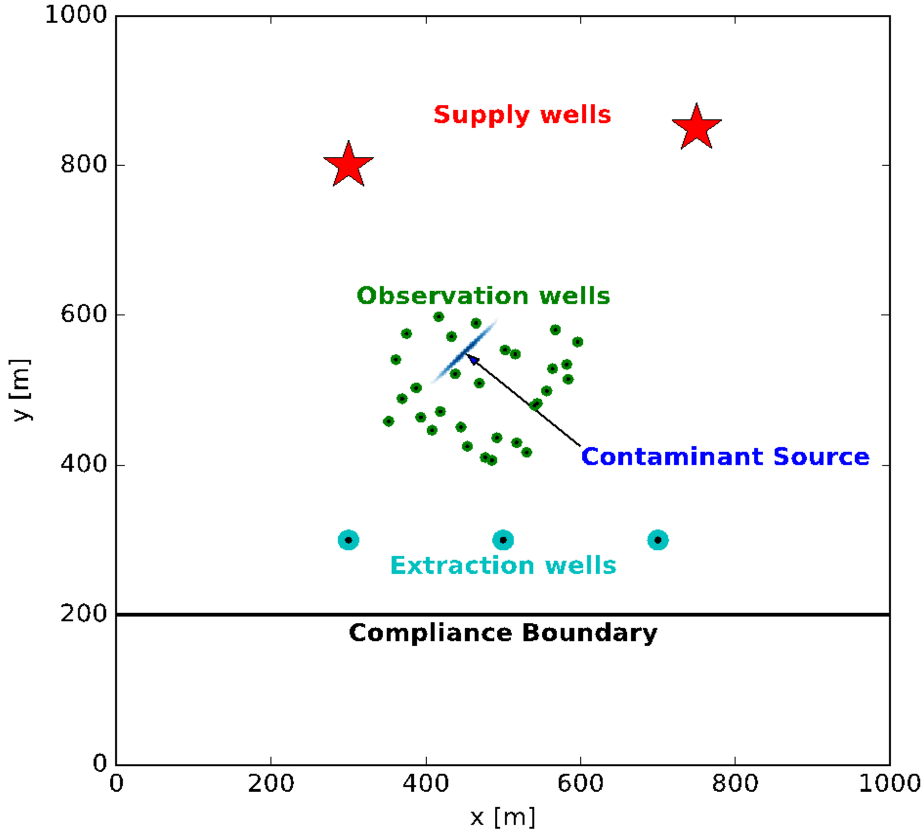

Fig. 2: Map of the representative site. The green dots denote the locations of wells that are used for monitoring the plume evolution, the red stars denote the locations of water supply wells, the cyan dots denote the locations of potential extraction wells, and the black line denotes the compliance boundary. Along the compliance boundary and further to the south, concentrations of the contaminant cannot exceed a specified threshold. The blue ellipse denotes the location where the contaminant enters the aquifer from the vadose zone.

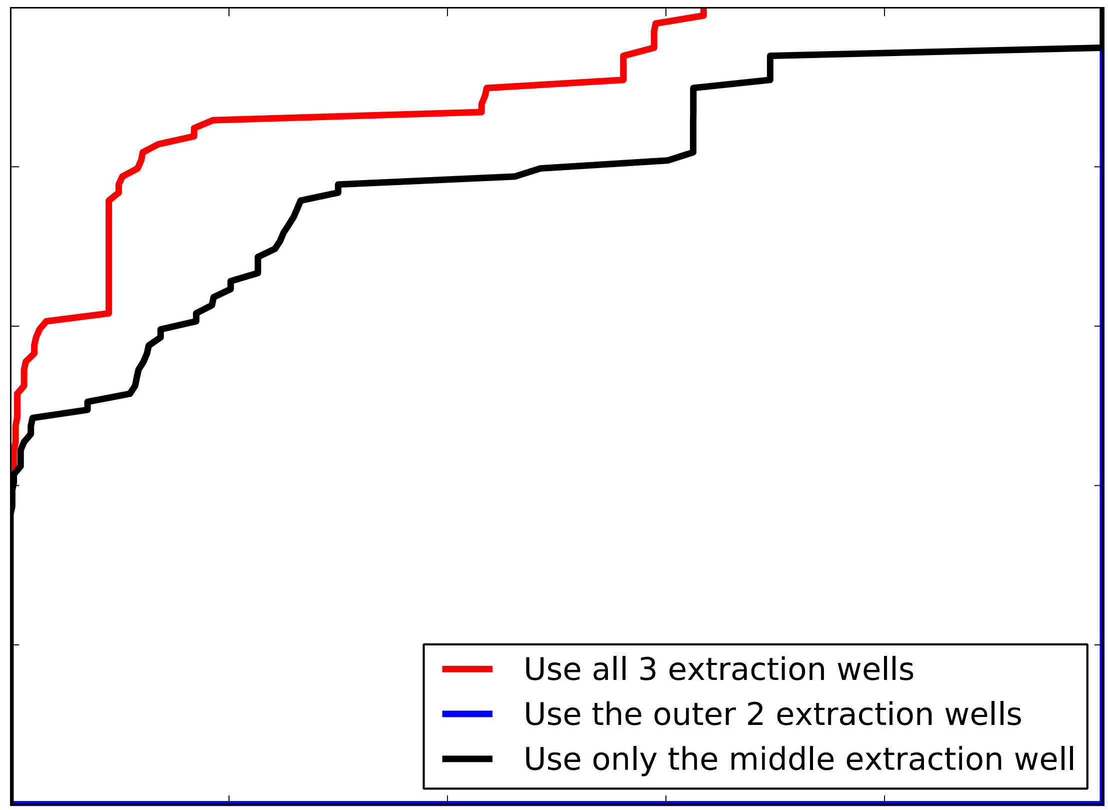

Fig. 3. For a given probability of failure, the robustness against uncertainty is shown for each of the three remedies considered. The robustness against uncertainty quantifies how wrong the modeler can be in the construction of the physical and probabilistic models while still ensuring that the probability of an undesirable outcome remains below the value on the x-axis.

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