Decision Analyses for Groundwater Remediation

Velimir V. Vesselinov, Daniel O’Malley, Danny Katzman

Los Alamos National Laboratory

Waste Management Symposium, March 7, 2017
LA-UR-17-21909
Decision analyses for Groundwater Remediation

- Robust and scientifically defensible decision analyses are critical for groundwater remediation
- Groundwater contamination is a significant national and international problem
- US National Research Council (NRC) recently estimated the liabilities associated with groundwater contamination in the US at over $100 billion
- US NRC also reports that over “90% of court mandated groundwater remediations fail”
  - We must perform better modeling and make better decisions
- Frequently these failures are due to “unanticipated complexities”
  - We must perform robust quantification of uncertainties impacting the remedial decisions
Challenges

- Scales
- Uncertainties
Subsurface contaminant plumes are spread over the kilometer scale

- Models must predict contaminant behavior at field scales

Contaminant behavior is driven by processes at pore scales

- Models must account for processes at pore scales

We cannot perform even a single model run that accounts for all processes at the field and pore scales

- Models must be capable to capture the most important processes: e.g., pore-scale mixing and field-scale spreading (dispersion)

Uncertainties are present at different scales

- Robust decision analyses tools are needed that would need to perform numerous model runs (high-performance computing)
Challenges: Probabilistic Uncertainties
Challenges: Non-probabilistic Uncertainties
Challenges: Uncertainties

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However, many environmental management uncertainties cannot be represented probabilistically.
Challenges: Uncertainties

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- For example, geologic heterogeneity is typically unknown (left die)

Decision Analyses

- BIG-DT
- LANL Chromium site
- BIG-DT Analysis
- MADS
Challenges: Uncertainties

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- We also do not know which model of heterogeneity is representative (right die), but we must choose a single representative model
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- We also do not know what all the sides of the dice look like, and how many sides there are
Challenges: Uncertainties

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▶ Therefore, we cannot enumerate all possible outcomes
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- We also do not know what all the sides of the dice look like, and how many sides there are
- Therefore, we cannot enumerate all possible outcomes
- All these issues make purely probabilistic (Bayesian) analyses flawed for many environmental-management problems (for example, using GoldSim)
Challenges: Uncertainties

- Many uncertainties at various scales
  - Model uncertainties (conceptualization and model implementation)
  - Parameter uncertainties
  - Data uncertainties (measurement errors)
  - Uncertainties in the performance of the engineered environmental management system
- All of these uncertainties can have both:
  - **probabilistic** components, and
  - **non-probabilistic** components
- We have developed a novel methodology and advanced computational tools that can address **probabilistic** and **non-probabilistic** uncertainties
- **BIG-DT**: Bayesian-Information Gap Decision Theory
- **MADS**: [http://mads.lanl.gov](http://mads.lanl.gov)
**Challenges**

- **Scales**: We have developed novel modeling tools accounting for small-scale processes in large-scale models.
- **Uncertainties**: We have developed novel decision analysis tools (Bayesian-Information Gap Decision Theory/MADS).
BIG-DT contaminant remediation problem: Scenario 1
BIG-DT contaminant remediation problem: Scenario 2
Known:
- 10 annual concentration observations at 19 wells (190 in total)
- Location of the compliance point

Estimated (probabilistic uncertainties):
- location, size, contaminant mass flux at the source
- aquifer flow properties (groundwater flow direction, magnitude, etc.)
- aquifer transport properties (porosity, dispersivity, etc.)

Unknown (non-probabilistic uncertainties):
- geochemical reaction rate (natural/enhanced)
- contaminant dispersion mechanism: classical (Fickian) or anomalous (non-Fickian)
BIG-DT results: Scenario 1

▶ To Act or Not to Act?

- Act = Perform Enhanced Attenuation (EA)
- Not to Act = Natural Attenuation (NA)

- To Act is the Answer

If we are very wrong about the geochemical reaction rates and the contaminant dispersion mechanisms, EA is the more robust option.
To Act or Not to Act? That is the Question.

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BIG-DT results: Scenario 2

- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)
  - Not to Act = Natural Attenuation (NA)
- Not To Act is the Answer

Even if we are very wrong about the geochemical reaction rates and the contaminant dispersion mechanisms, both NA and EA provide similar results.
BIG-DT results: Scenario 2

▶ To Act or Not to Act? That is the Question.
  ▶ Act = Perform Enhanced Attenuation (EA)
  ▶ Not to Act = Natural Attenuation (NA)
▶ Not To Act is the Answer

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LANL Chromium site

Los Alamos National Laboratory

LANL Chromium plume

San Ildefonso Pueblo
Model predicted drawdowns caused by the water-supply pumping

Time=2010.42
Chromium bio-remediation modeling (ChroTran)

**Decision Analyses**
- BIG-DT
- LANL Chromium site
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Time=29 (d)

**Variables**
- Free_food
- biomass
- Cr(VI)

**Color Scales**
- Max: 292.7
- Min: 9.000e-31
- Max: 9.966e+06
- Min: 3.000e-14
- Max: 10.00
- Min: 5.807e-14
Geochemical particle-based modeling

- \( A + B = C \)
- \( X + Cr^{6+} = Cr^{3+} \)
- Reduction of contaminant \( B \) by injecting \( A \)
- Reduction of contaminant \( A \) by interacting with \( B \)
- \( A \) instantaneously released (500 moles)
- \( B \) uniformly distributed in the aquifer (1000 moles)
20% of A did not react.
Bayesian Information Gap Decision Analysis: Setup

**Unknowns:**
- contaminant mass release, source location \((x, y)\) and size
- hydraulic conductivity
- porosity
- dispersivity (longitudinal and transverse)
- contaminant transport parameters (mean mobile/immobile times of pore-scale mixing)

**Knowns:**
- well locations
- well pumping rates
- ambient hydraulic gradient
- location of compliance boundary
- hydraulic heads at the monitoring wells
- contaminant concentrations at the monitoring wells
- 30 monitoring wells
- 10 annual observations (heads/concentrations) per well (600 in total)
Bayesian Information Gap Decision Analysis: Pumping

Decision Analyses
BIG-DT
LANL Chromium site
BIG-DT Analysis
MADS
Bayesian Information Gap Decision Analysis: Results

- **Use all 3 extraction wells**
- **Use the outer 2 extraction wells**
- **Use only the middle extraction well**
MADS is an open-source high-performance computational framework.

MADS implements a wide range of state-of-the-art and novel advanced computational techniques for big-data and complex model analyses (including machine learning).

MADS provides tools for coupling with any existing physics simulator (FEHM, Amanzi, PFloTran, ChroTran, etc.)

MADS source code, examples, test problems, performance comparisons, and tutorials are available at:

- http://mads.lanl.gov
- http://madsjulia.github.io/Mads.jl
MADS has applied to perform various types of data- and model-based analyses related to the LANL chromium site:

- Contaminant source identifications
- Contaminant source characterizations (using models and machine learning)
- Monitoring network designs
- Optimization of injection/extraction well locations for hydraulic plume control
- Sensitivity analyses
- Uncertainty quantifications
- Evaluation of remediation scenarios
- Decision analyses
In the last 10 years, model analyses have accumulated more than 1,000 CPU-years of computational time utilizing simultaneously up to 4,096 processors on the LANL HPC clusters.

... so far, all the blind model predictions (estimates/uncertainties) have been generally consistent with the new site observations.