Reproduction of a Complex Tracer Test through Explicit Simulation of a Heterogeneous Aquifer using Bayesian Markov Chain Monte Carlo

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Abstract Simulation of tracer response curves in waste rock systems can be difficult using conventional numerical techniques, due to the presence of local heterogeneities. Instead, alternative methods are required that can explicitly handle the inhomogeneous nature of flow. Such an approach is presented herein that couples sequential Gaussian simulation with Bayesian inference using a Markov Chain. Results show that complex tracer behaviour can be reproduced using simple, spatially conditioned, Markov Chains. Additionally, external conditioning routines are found to be more efficient in controlling Markov state transition compared to random resampling or collocated cokriging.

Key words Tracer Test, Geostatistics, Bayesian, Waste Rock, Markov Chain

Introduction

The basic conceptual model for backfill into a previously mined out open pit is that of a relatively homogeneous, coarse-grained, granular media with some degree of anisotropy in hydraulic conductivity due to the mechanics of the backfill process. While this model is a reasonable starting point, flow behaviour in real world systems is often more complex due to the variability in dump emplacement.

Much like depositional facies in a sedimentary environment, backfilled pits display particle segregation resulting in interbedded layers forming along the angle of repose. The degree of segregation is a direct result of the style of dump emplacement, which is affected by such factors as lift height, initial gradation, and placement technique (BCMWRPRC 1991). Generally, the greater the lift height, the more segregation occurs with larger particles displaying longer run-outs. The end result is a fining upward sedimentary sequence, which can have a relatively simple or highly complex spatial distribution.

Characterization of the hydraulic behaviour of such backfilled systems often occurs through multi-stage field programs. Early stage testing may involve slug and/or pump testing, which while providing larger-scale equivalent hydraulic properties, is often unable to deconvolute the intricacies of highly heterogeneous flow systems. This is where subsequent stage tracer testing can be useful, as it can confirm the presence of and help delineate heterogeneities in the backfill.
Recent bromide tracer testing in such a backfilled dump has shown the heterogeneous nature of such systems, with tracer behaviour displaying a highly complex plume distribution (Figure 1). Reproduction of such behaviour proved difficult using conventional numerical modelling techniques, which were unable to reproduce the plume using simple conceptual model setups. Instead, a coupled Bayesian inference and geostatistical approach was ap-

plied (Irving and Singha 2010; Mariethoz et al. 2010). This involved construction of a random series of heterogeneous hydraulic conductivity (K) and porosity (n) fields, which were assessed based on their conditional probability of reproducing the measured bromide concentration curves.

Field Observations

Tracer testing was conducted using a dipole configuration, whereby water extracted from the pumping well was directly reinjected into the injection well forming a continuous loop (Figure 1). Water was cycled at a constant rate of 546 m³/day. During the first 22 days of the test, bromide tracer was added to the reinjected water at an average concentration of 34.7 mg/L. This was followed by passive cycling and monitoring for an additional 87 days (i.e. water from the pumping well was re-injected without any bromide added). Bromide concentration curves were monitored at the pumping well (PW) and four waterloo sampling ports (WP1-4).

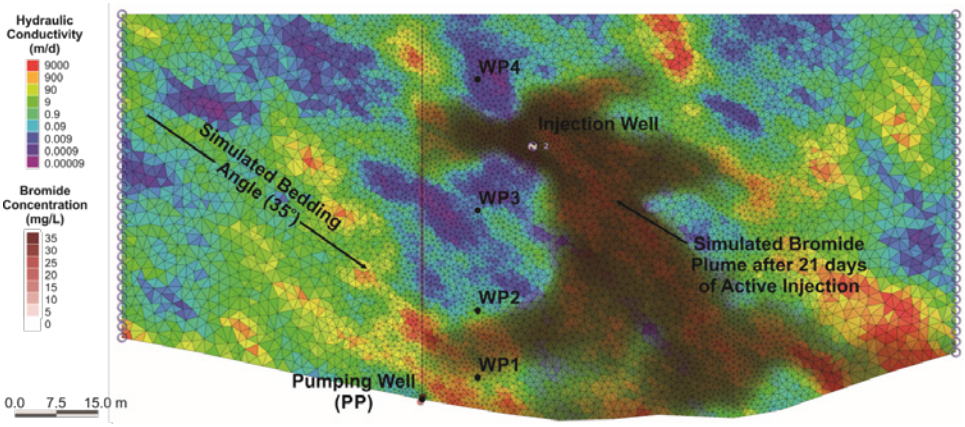

Figure 1 *Two-dimensional groundwater flow setup in FEFLOW. Simulated bromide plume and random K field are presented for the highest probability model generated using the external conditioning approach.*

Results of the tracer test showed appreciable amounts of tracer only in the deepest part of the flow system (PP and WP4), while the upper most zones nearest the injection horizon displayed minimal (WP2) to no response (WP3 and WP4). This odd response behaviour was unexpected, and suggested that the dump emplacement is far more heterogeneous then pre-test homogeneous models suggested.

Methodology

Numerical Groundwater Simulation Model

Numerical groundwater modelling has been completed using the modelling software FEFLOW (DHI 2016). A two-dimensional planar model was setup through the current backfilled pit (Figure 1). Groundwater flow behaviour was modelled assuming saturated, steady-state conditions; while transport modelling was conducted under transient conditions. Left

and right edges of the model were set as constant head boundaries. The top and bottom boundaries were simulated using no-flow (zero-flux) conditions. Dipole pumping was simulated using two coupled constant flux boundaries with the rate adjusted to match the measured head observed in the injection well. Active tracer injection was simulated using a constant concentration boundary set to an average valve of 34.7 mg/L for the first 21.5 days. This was followed by linking of the pumping and injection well concentrations to simulate passive dipole cycling for the remaining 87.5 days.

Geostatistical Simulation

Random generation of the heterogeneous hydraulic conductivity and porosity fields were conducted using sequential Gaussian simulation (SGS; Deutsch and Journel 1998). The approach works by sequentially generating random variates within a set of grid nodes based on Gaussian deviations from a stationary mean. Heterogeneity is imposed through the conditioning of local probability distributions using simple kriging routines, with the heterogeneous structure defined by vario- and/or correlograms. The sequential generation sequence is randomized between trials using a random walk. The end result is a random realization of a continuous variable which matches the underlying spatial structure of said variable.

Bayesian Markov Chain Monte Carlo

Estimation of the *in-situ* heterogeneity structure was conducted using Bayesian inference, with FEFLOW models assessed based on their conditional probability of reproducing the measured bromide behaviour. Specifically, models were assessed using Bayes' Theorem:

$$P(x|\theta)=\frac{P(\theta \vee x)P(x)}{P(\theta)} \qquad \text{Equation 1}$$

where:

- $P(x \vee \theta)$ is the posterior distribution or conditional probability that the model state (i.e. heterogeneous random field) is representative of the tracer response behaviour.
- $P(\theta \vee x)$ is the conditional probability that the model matches the observed tracer behaviour given the simulated model state (i.e. random field).
- $P(x)$ is the prior probability, or one's belief before conducting the modelling that the simulated heterogeneous structure is representative of the *in-situ* conditions.
- $P(\theta)$ is a normalization constant related to the modelling errors.

In practice, the direct solution of Bayes' Theorem is often difficult, owing to the calculation of $P(\theta)$ which requires prior knowledge of model errors. Instead, it is often easier to approximate the equation using a Monte Carlo solution, such as Markov Chain Monte Carlo (MCMC). The approach works by setting up a Markov chain, which has an equilibrium distribution that matches the desired posterior distribution ($P(x|\theta)$). One method of setting

up such a chain is the Metropolis algorithm (Metropolis et al. 1956). The approach involves a five step procedure:

1. Initialize a random heterogeneous state (x_{old}).
2. Randomly generate a new state (x_{new}) from the old state (x_{old}) based on a symmetric, transitional jump function (typically a Gaussian distribution).
3. Calculate the acceptance ratio (α):

$$\alpha = min\left[1, \frac{L\left(\theta \middle| x_{new}\right) P\left(x_{new}\right)}{L\left(\theta \middle| x_{old}\right) P\left(x_{old}\right)}\right] \qquad \text{Equation 2}$$

4. Randomly select a uniform value (u) between 0 and 1:
   a. If $u \leq \alpha$ move to the new state ($x_{old} = x_{new}$), else
   b. If $u > \alpha$ remain in the current state ($x_{old} = x_{old}$)
5. Restart the algorithm at step 2.

In order to limit the impact of the random starting position, an initial *N* states are discarded at the start of the sequence (known as the burn-in period), while the algorithm converges on the high probability space. Once the burn-in period is complete, samples are saved every N steps, with interstitial steps discarded to limit autocorrelation effects. The process is repeated until the desired sample size is reached.

Misfit Function

Definition of a misfit function is required in order to assess the conditional likelihood that the current model state (i.e. random field) is representative of the *in-situ* groundwater conditions. This was conducted by assuming independent, normally distributed data errors, resulting in the conditional likelihood being defined by (Mosegaard and Tarantola 2005):

$$L\left(\theta \vee x\right) = \exp\left(\frac{-\sum\left(\theta_{mod} - \theta_{obs}\right)^2}{\sigma^2}\right) \qquad \text{Equation 3}$$

where θ_{mod} and θ_{obs} are the calculated and measured response curves, and σ^2 is the standard deviation in the data errors.

Combined Model Structures

The above methodology was incorporated into FEFLOW using IFM programming (Figure 2). Transition between Markov states was controlled using three separate algorithms. These include:

1. **Random resampling:** during each iteration of the Markov chain a random

subset of the model elements were regenerated using the SGS code (Irving and Singha 2010).

2. Collocated cokriging: the new state was cokriged from the previous state, with

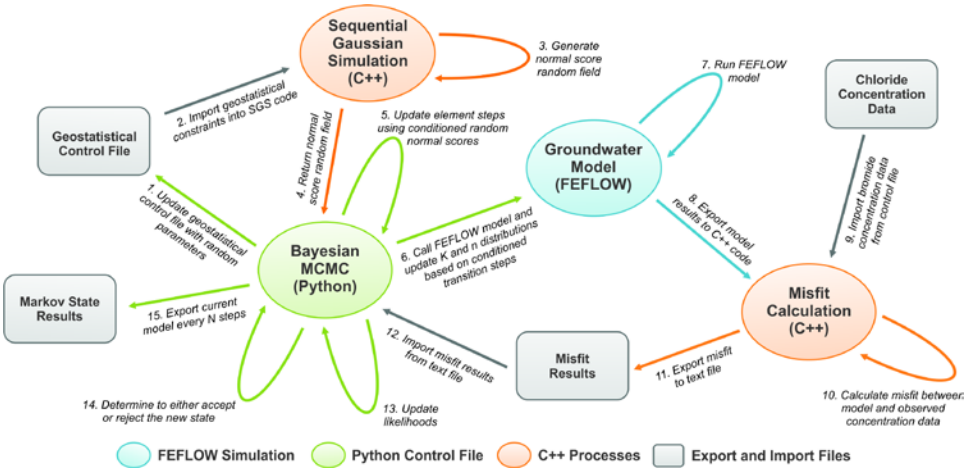

Figure 2 *Overview of model structure using external conditioning approach.*

the transition controlled using a correlation coefficient (Xu et al. 1992).

3. **External conditioning:** each element was treated using a unique set of variables (K, n), with transition between the states controlled using individual Gaussian jump functions. Spatial conditioning is imposed by conditioning the Gaussian jumps based on the jumps of nearby neighbours using SGS.

In a well constrained Markov chain the jump size should be optimized to ensure efficiency in the model solution. A chain with a jump that is too small will mix poorly, and be inefficient at converging on the high probability space; while too large of a jump will have a poor acceptance rate again resulting in poor mixing and convergence. Roberts et al. (1997) showed that for single-variate Gaussian solutions the target acceptance rate should be 50% to optimize chain convergence towards high probability space. This drops to 23% for *N*-dimensional Gaussian distributions.

Prior Information

Before initiating the Markov Chain process, the SGS generator needed to be setup to allow for construction of Markov states. This was done by reviewing field data, published literature, and best engineering judgement, in order to define the input parameters.

Backfill sedimentary sequencing was simulated using three key parameters: bedding angle, anisotropy factor, and spatial continuity. The bedding angle was set to the angle of repose (35^{o}). Due to the relatively unknown nature of the anisotropy factor and spatial continuity, uniform priors were assumed, which varied between 1^{x} to 3^{x} and 2 to 20 m respectively.

Prior porosity information was available from downhole nuclear magnetic resonance (NMR) testing in the observation well. Results of the NMR analysis indicate a mobile water fraction (effective porosity) of 0.276, with a standard deviation of 0.08.

Large-scale hydraulic conductivity estimates were available from a prior pump test conducted in the injection well. Estimates of the hydraulic conductivity indicate a mean valve of 436 m/d. Small-scale variability in the conductivity was estimated from NMR results, which suggest a log-transformed standard deviation between 0.35 to 1.71 orders of magnitude. A vertical trend in the hydraulic conductivity was simulated to reproduce grain size segregation associated with dump emplacement. The trend was assigned based on a uniform distribution between one and three orders of magnitude across the saturated thickness.

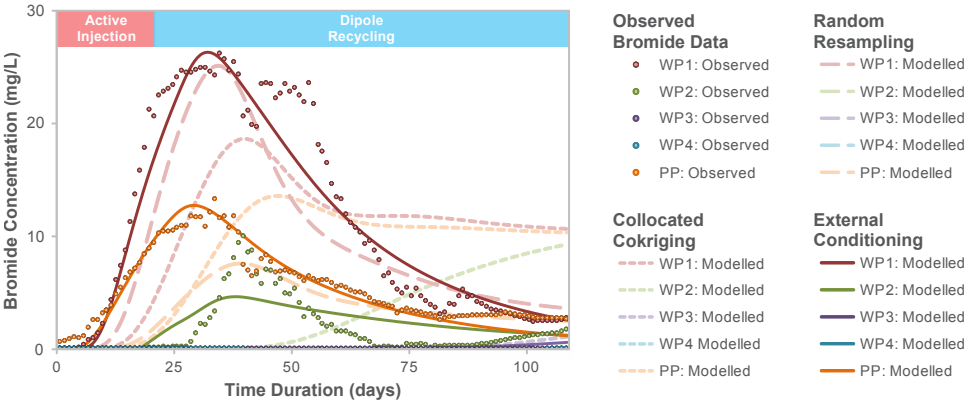

Figure 3 *Comparison of highest probability models with observational data.*

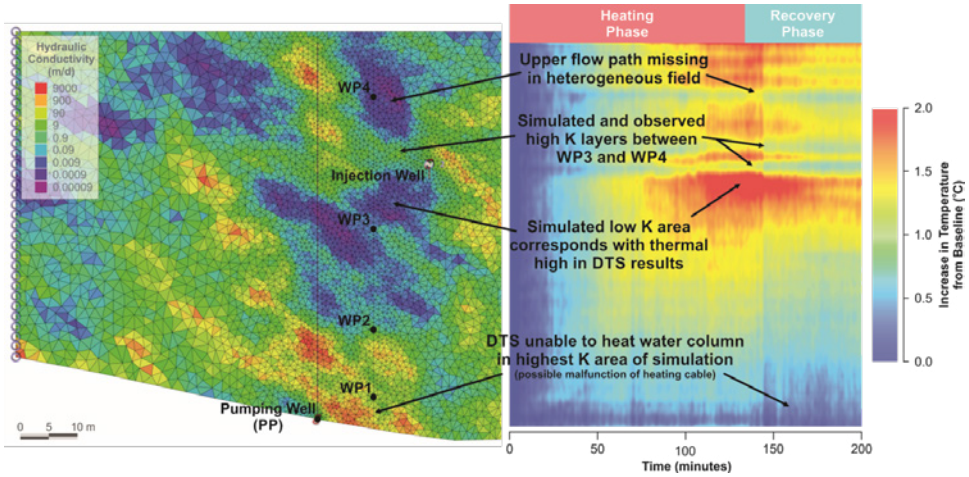

Figure 4 *Comparison of highest probability random field, generated using external conditioning method, with distributed temperature sensing (DTS) results.*

Stochastic Results and DiscussionThe three tested Markov transition algorithms showed varying degrees of success in converging on the high probability space. Initial results using the random resampling approach showed promise during the initial burn-in period, with acceptance rates near 30%; however rates soon dropped below 2% as the model misfit approached 14,000 $(mg/L)^2$ (Figure 3). The percentage of the model resampled was varied between 90 and 99%, but acceptance rates did not improve significantly, likely due to the small number of elements resampled during each iteration.

Collocated cokriging routines were found to have improved convergence compared to random resampling, with models converging on a higher probability space after an initial 24 hour run (4,000 mg/L2; Figure 3). The improved convergence was likely associated with the complete resampling of all elements between Markov states. Correlation coefficients were varied between 0.8 and 0.999, with improved acceptance rates (40%) found when using higher correlation coefficients (0.999). Convergence was found to flat-line near a misfit of 4,000 mg/L^2 with minimal model improvement during subsequent runs.
The final attempted transition algorithm, external conditioning, was found to be the most efficient at convergence on the high probability space. Model misfits were found to drop from an initial starting value 26,000 mg/L^2 to a minimum of 1,700 mg/L^2 after less than 12 hours, or 3,000 model runs. Subsequent simulations showed further convergence with a minimum value of 1,000 mg/L^2 after 25,000 trials (Figure 1, Figure 3). Acceptance rates remained high even in higher probability space, with rates near 27%. Gaussian jumps were set to 1.3% and 13% of the standard deviation in the K and n parameters, respectively.

As a validation step, random fields generated using the external conditioning algorithm were compared to distributed temperature sensing (DTS) field results. DTS tests allow for flow-path characterization by heating a well column and then monitoring the recovery to baseline (Banks et al. 2014). Areas of higher hydraulic conductivity are more difficult to heat and recover quicker compared to lower conductivity zones. A visual comparison between the DTS and Bayesian-MCMC results indicate a reasonable agreement between the two independent methods (Figure 4).

Conclusions and Future Work

Heterogeneity is an intrinsic property of waste rock systems; however, such attributes are typically overlooked when systems are modelled using larger-scale equivalent porous media properties. While this is often appropriate for calibration of models to pump tests, it can fail to recognise the nuances of waste rock deposition. Bromide response behaviour presented herein has shown that local-scale flow dynamics can be heavily influenced by this depositional history. Early results have shown that the coupling of Bayesian-MCMC approaches with geostatistical routines can provide an effective approach to simulate such heterogeneity. Additionally, the approach was found to have improved convergence when Markov state transition was controlled by external conditioning routines, as opposed to random resampling or collocated cokriging. Research remains on-going with additional model runs being conducted to further explore the probability space.

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