

## Improved inverse modeling for flow and transport in subsurface media: Combined parameter and state estimation

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[1] Current approaches for inverse modeling (IM) to estimate flow and transport properties in subsurface media implicitly assume that uncertainty in the input-output representation of the model arises from uncertainty in the parameter estimates. However, uncertainties in the modeling procedure stem not only from uncertainties in the parameter estimates, but also from measurement errors, from incomplete knowledge of subsurface heterogeneity, and from model structural errors arising from the aggregation of spatially distributed real-world processes in a mathematical model. In this paper we present an improved concept for IM of subsurface flow and transport. Studies using interwell reactive tracer test data demonstrate that this new method, called Simultaneous Optimization and Data Assimilation, results in parameter estimates and model prediction uncertainty bounds which more closely mimic the properties of the subsurface. Most important is the finding that explicit treatment of input, output and model structural errors during IM, significantly alters the optimal values of the model parameters. **Citation:** Vrugt, J. A., B. A. Robinson, and V. V. Vesselinov (2005), Improved inverse modeling for flow and transport in subsurface media: Combined parameter and state estimation, *Geophys. Res. Lett.*, 32, L18408, doi:10.1029/2005GL023940.

### 1. Introduction and Scope

[2] While considerable progress has been made in the development and application of Inverse Modeling (IM) to estimate subsurface flow and transport properties, current methodologies are known to suffer from a lack of rigor in treating various sources of error [Katul *et al.*, 1993; Parlange *et al.*, 1993; Vrugt *et al.*, 2005]. Automated IM codes generally compute parameters and their uncertainty ranges as though model-data mismatches are solely attributable to parameter uncertainty. Unfortunately, other errors, such as those arising from inadequate representation of physical processes have not been handled in an explicit manner. This can lead to unrealistically small parameter uncertainty estimates, and overconfident predictions when the model is used in forecasts of future behavior.

[3] In the past few years, ensemble-forecasting techniques based on Sequential Data Assimilation (SDA) methods have become increasingly popular due to their potential ability to explicitly handle the various sources of uncertainty in geophysical modeling. Techniques based on the Ensemble Kalman Filter (EnKF) [Evensen, 1994] have been suggested as having the power and flexibility required for data assim-

ilation using nonlinear models. In particular, Vrugt *et al.* [2005] recently presented the Simultaneous Optimization and Data Assimilation method (SODA), which uses the EnKF to recursively update model states while estimating time-invariant values for the model parameters using the Shuffled Complex Evolution Metropolis stochastic-ensemble optimization approach (SCEM-UA) [Vrugt *et al.*, 2003]. A novel feature of SODA is its explicit treatment of errors due to parameter uncertainty, uncertainty in the initialization and propagation of state variables, model structural error, and output measurement errors.

[4] In this letter, we demonstrate the usefulness and applicability of SODA for improved IM of flow and transport properties in subsurface media. To illustrate our approach, we consider the interpretation of an interwell tracer experiment conducted in fractured tuff, showing how the method yields more reliable field-scale sorption parameters and uncertainty estimates.

### 2. Methods

[5] Consider a model  $\Phi$  in which the time evolution of the state vector  $\psi$  is described with:

$$\psi_{t+1} = \Phi(\psi_t, \tilde{X}_t, \theta) \quad (1)$$

where  $\tilde{X}$  represents the observed forcing,  $\theta$  is a parameter set, and  $t$  denotes time. These model states are related to the model output prediction,  $y_t$  according to:

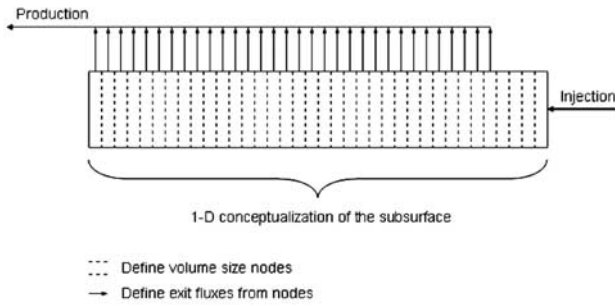
$$y_t = H(\psi_t) \quad (2)$$

where the operator  $H(\cdot)$  maps the state space into the measurement or model output space.

[6] The classical approach to determine the values of  $\theta$  in Equation (1) is by minimizing the following simple least squares (SLS) objective function with respect to  $\theta$ :

$$F_{SLS} = \sum_{t=1}^n w_t (y_t - \tilde{y}_t)^2 \quad (3)$$

where  $w_t$  denote the weights for particular data points and  $\tilde{y}_t$  represent the observations available at time steps  $1, \dots, n$ . This approach, which neglects input errors and lumps observed response and model structural error into one single white noise term, has serious shortcomings: the best-fit parameter estimates so determined represent the optimization algorithm's best attempt to trade off input, output and model structural error, while the parameter uncertainty estimates reflect the sensitivity of  $F_{SLS}$  to parameter deviations. The connection of these parameters to underlying properties of the medium is tenuous.



**Figure 1.** Schematic overview of the conceptual mixing model used for characterization of the subsurface. The arrows denote the side exits to reproduce the known Residence Time Distribution of Bromide.

[7] In response to these issues, *Vrugt et al.* [2005] recently proposed the combined use of parameter optimization and sequential data assimilation (the SODA algorithm) to facilitate improved treatment of input, output, parameter and model structural errors in hydrologic modeling. The SODA method implements an inner Ensemble Kalman Filter (EnKF) loop for recursive state estimation (conditioned on an assumed parameter set), within an outer stochastic global optimization loop for batch estimation of the posterior density of the parameters. The EnKF uses a Monte Carlo based ensemble of state trajectories to propagate and update estimates of the mean and covariance of the uncertain state variables from one time step to the next. When an output measurement is available, each forecasted ensemble state vector is updated by means of a linear updating rule in a manner analogous to the Kalman Filter. A detailed description of the SODA method, including the algorithmic details is found in work by *Vrugt et al.* [2005] and so will not be repeated here. In the next section we discuss the particular implementation details for our current case study.

### 3. Case Study: Reactive Tracer Experiment

[8] The SODA method is applied to the analysis of a 127-day interwell reactive tracer experiment conducted at the C-wells near Yucca Mountain, Nevada. The purpose of this and other similar tests at this site was to establish the validity of transport models and laboratory-determined sorption parameters when applied to the saturated zone beneath the proposed Yucca Mountain nuclear waste repository. Forced-gradient, cross-hole tracer tests were conducted involving a nonsorbing solute tracer (bromide) and a weakly sorbing solute tracer (lithium ion). A comparison of breakthrough curves at the production well for Li and Br provides a means for estimating the subsurface properties for predictive modeling of radionuclide transport. A detailed description of the tracer test methods and initial interpretation appears in work by *Reimus et al.* [2003]. In this letter we restrict attention to the estimation of sorption isotherm parameters using the SODA method, comparing these results to a more traditional IM method.

[9] The numerical analysis is based on a model that uses a Residence Time Distribution (RTD) based interpretation of the mixing patterns in residence-time space. The method uses the RTD for the conservative Br tracer to construct a

one-dimensional conceptual mixing model of the subsurface for the sorbing tracer breakthrough curve. *Robinson and Viswanathan* [2003] showed how to build this advection flow path with side exits, called a micromixing model, and assign the locations and flow rates of the side exits to reproduce a given RTD (see Figure 1). The model forecasts the concentration at the production well,  $C_{t,out}$  at time step  $t$  as:

$$C_{t,out} = \frac{\sum_{i=1}^N C_{t,i} \cdot q_i}{\sum_{i=1}^N q_i} \quad (4)$$

where  $q_i$  represent the exit fluxes,  $N$  is the number of nodes, and  $C_i$  denote the simulated nodal concentrations of the respective tracer. Instead of requiring the collection of complex, in situ information on the three-dimensional subsurface flow pathways, the method ensures that the correct RTD for the conservative tracer is reproduced. Then, the reactive tracer is modeled in the same flow path by including sorption using a Freundlich sorption isotherm:

$$S_{t,i} = K_f C_{t,i}^n \quad (5)$$

where  $S$  and  $C$  are the sorbed and aqueous concentrations at node  $i$ , respectively, and  $K_f$  and  $n$  are sorption parameters that need to be estimated by modeling the Li breakthrough curve. These parameters are assumed to be constant along the flow path, making the sorption behavior independent of residence time. The computer code FEHM [*Zyvoloski et al.*, 1997; *Robinson et al.*, 2000] was used to perform the flow and reactive transport calculations.

[10] In our state-updating scheme, the mismatch between the measured and simulated Li concentrations at the production well (left hand side in Figure 1) is used to recursively update the concentrations of the FEHM simulated Li concentrations,  $C_{t,i}^-$  within each node. The updated concentration,  $C_{t,i}^+$  at each node is computed as:

$$C_{t,i}^+ = C_{t,i}^- + K_{t,i} \cdot \frac{Z_{t,i} \cdot (C_{t,out}(\theta) - \tilde{C}_{t,out}) \cdot \sum_{i=1}^N q_i}{q_i} \quad (6)$$

where  $K_{t,i}$  denotes the Kalman Gain,  $Z_{t,i}$  is the relative contribution of node  $i$  in simulating  $C_{t,out}$  (the total outlet concentration), and  $\tilde{C}_{t,out}$  represents the measured Li outlet concentration at time step  $t$ . The Kalman Gain is computed as:

$$K_{t,i} = \left( 1 - \frac{\text{var}[\tilde{C}_{t,out}]}{\text{var}[C_{t,out}]} \right) \quad (7)$$

The variance of the measurement error,  $\text{var}[\tilde{C}_{t,out}]$  was assumed homoscedastic and estimated using a non-parametric time-difference approach [*Vrugt et al.*, 2005], whereas the size of the total error,  $\text{var}[C_{t,out}]$  was estimated each time FEHM is evaluated against the observations. This total error is, therefore, conditional on the specific parameter set used in each ensemble run. This total error term is the sum of measurement, input and model error,

**Table 1.** Description of the Model Parameters Subject to Calibration, Including Their Prior and Posterior Uncertainty Ranges Derived With the SCEM-UA and SODA Method

| Par.  | Unit                      | Description        | Prior     | Posterior |           |
|-------|---------------------------|--------------------|-----------|-----------|-----------|
|       |                           |                    |           | SCEM-UA   | SODA      |
| $K_f$ | [ppm <sup>1-n</sup> cc/g] | Sorption parameter | 0.00–1.00 | 0.28–0.32 | 0.53–0.88 |
| $n$   | [–]                       | Sorption parameter | 0.00–1.00 | 0.63–0.64 | 0.45–0.49 |

which itself consists of conceptual errors, process uncertainty, and process misrepresentation. Although, in principle all of the errors terms that make up the model error could be handled separately, in the absence of compelling information about the size of the individual terms, we decided to lump them together in a single model error estimate. Based on recommendations in the classic treatise of the EnKF in work by Evensen [1994], the time evolution of the model error was modeled as a first-order autoregressive process.

[11] For parameter estimation a Bayesian density criterion is specified that measures the “closeness” between the (EnKF derived) mean ensemble model forecast,  $\bar{C}_{t,out}(\theta)$

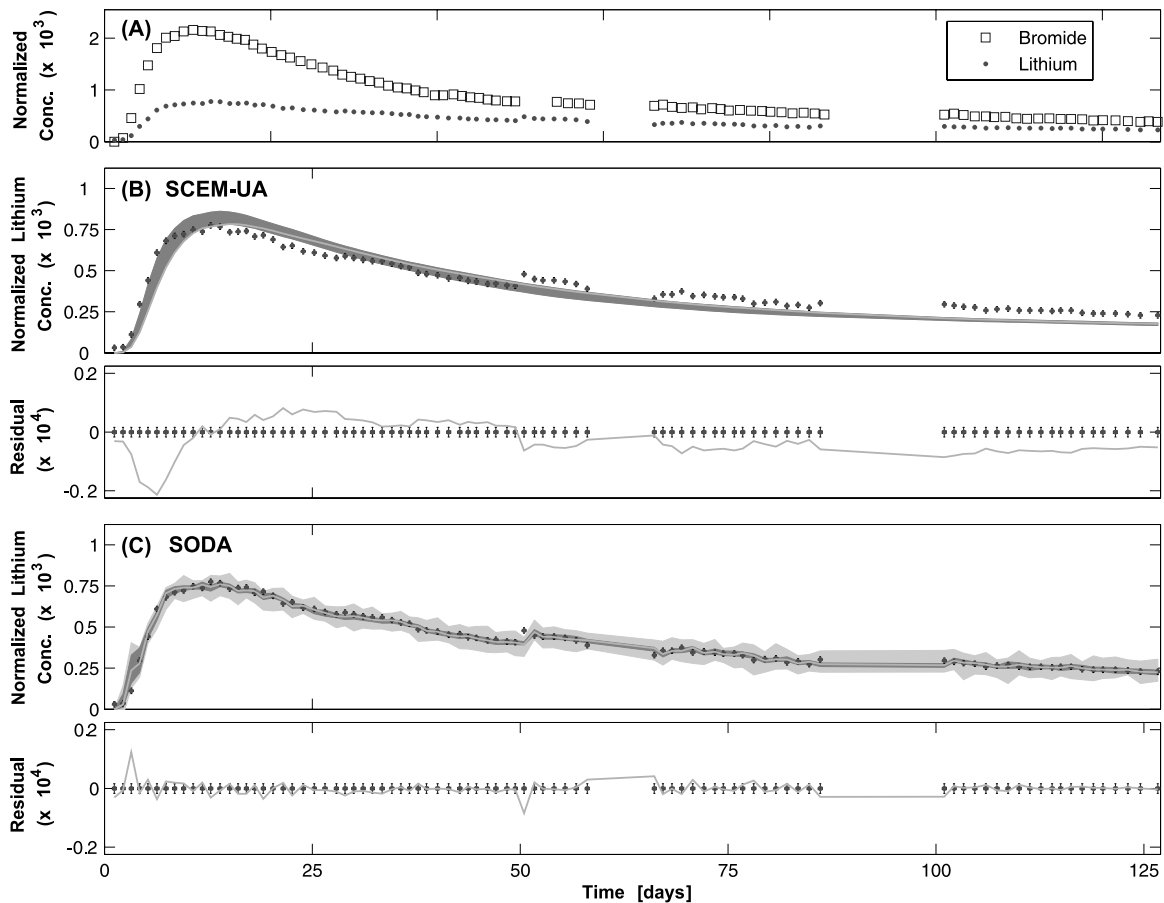
and the corresponding measurement, resulting in the posterior density function:

$$p(\theta|\tilde{Y}) \propto \sum_{t=1}^n [\bar{C}_{t,out}(\theta) - \tilde{C}_{t,out}]^{-n} \quad (8)$$

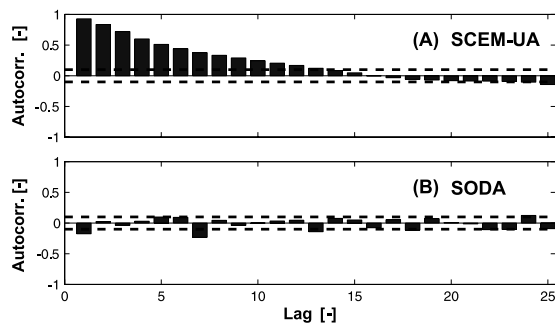
To generate samples corresponding to the distribution in Equation (8), we use an implementation of the general-purpose Shuffled Complex Evolution Metropolis (SCEM-UA) global optimization algorithm, which provides an efficient estimate of the posterior distribution and its mode within a single optimization run [Vrugt et al., 2003]. Table 1 summarizes the calibration parameters and their prior uncertainty ranges.

#### 4. Simulation Results and Discussion

[12] A distributed computing implementation of the SODA algorithm was used to estimate field scale sorption parameters. A parameter search population of 100 points, in combination with 5 parallel sequences and 100 ensemble members was selected. The procedure used about 1,000 parameter evaluations to converge to a reasonable estimate



**Figure 2.** (a) Tracer test data from Reimus et al. [2003], (b) lithium breakthrough curve model predictions using a conventional SCEM-UA calibration (no state updating) and (c) the SODA calibration. Box plots denote the measurement uncertainty. In each case, the prediction given by the “best” parameter set is indicated using a solid black line and the prediction uncertainty bounds associated with the parameter estimates are indicated by the dark gray region. For SODA the additional uncertainty due to model error is indicated by the light gray region.



**Figure 3.** Autocorrelation functions of the time series of error residuals using (a) the SCEM-UA algorithm without state variable updating and (b) the SODA framework. The dashed lines denote the theoretical upper and lower 99% significance intervals of a time series of white residuals.

of the optimal model parameters, including their underlying posterior distribution. The results of this analysis are summarized in Table 1 and Figures 2 and 3 and discussed below.

[13] Figure 2a shows the measured breakthrough curves of Br and Li, scaled to the relative mass of each tracer injected, and Figure 2b shows a classical IM parameter estimation, *without state variable updating*, using the SCEM-UA optimization algorithm. The dark gray region represents the uncertainty in the FEHM model predictions associated with the uncertainty in the parameter estimates. The box plot symbols are used to denote the median, lower and upper quartile values of the confidence intervals for the measured  $\text{Li}^+$  breakthrough curve. Notice that although the model captures the general trends in the data, the residuals exhibit considerable variation in bias, variance and correlation structure. The simulated 99% confidence intervals for the Li concentrations at the production well are clearly too narrow and do not include all of the measured concentrations, indicating that the estimation procedure is placing too much confidence in the validity of the mixing model. Figure 2c shows the results for IM with the SODA approach. The simulated overall 99% confidence intervals of the Li breakthrough curve, representing both parameter (dark gray) and state variable uncertainty (light gray) caused by model structural and input errors are now reasonable and tend to bracket the observations.

[14] Table 1 reports the posterior parameter distributions for the SCEM-UA and SODA cases. First, notice that the estimated parameter values are quite different for the two cases. If the model structure were correct and there were no errors in the input and output data, no state adjustments would be needed during IM, and the SCEM-UA and SODA method would identify the same mode of the posterior distribution. Not properly accounting for input and model structural error leads to corrupted parameter estimates, which are compensating for these errors. Second, the parameter uncertainties for the SODA case are much wider. Adopting a strategy of recursive state adjustments eliminates the bias that yields artificially low uncertainty estimates for the SCEM-UA case. Thus, the SODA-derived uncertainties are more realistic and, we believe, more useful for flow and transport model predictions.

[15] This view is further supported in Figure 3 by comparison of the autocorrelation functions of the SCEM-UA and SODA derived time series of residuals. Autocorrelation is a measure of the accuracy of the model predictions. When performing a traditional IM using the SCEM-UA algorithm, there is significant autocorrelation between the residuals at the first few lags, confirming our earlier findings in Figure 2. By comparison, there is considerably less autocorrelation between the forecasted residuals using the SODA framework, suggesting that recursive state adjustments remove a large part of the bias in the FEHM model predictions. Finally, we note that the SODA derived uncertainty ranges of the Freundlich sorption isotherm are of similar order as the spatial variability encountered from laboratory experiments using different tuffs at the Yucca Mountain field site [Anghel *et al.*, 2002]. A further comparison with laboratory measurements is outside the scope of the current paper, but will be the subject of future research.

## 5. Conclusions

[16] In this paper, we have presented a combined parameter and state estimation method called Simultaneous Optimization and Data Assimilation (SODA) that results in improved IM for subsurface flow and transport. The method merges the strengths of the Ensemble Kalman Filter for recursive data assimilation to update model states, and the Shuffled Complex Evolution Metropolis algorithm for batch parameter estimation. Inverse modeling of interwell reactive tracer data demonstrates that the SODA approach results in more representative parameter uncertainties and associated model prediction uncertainty ranges. The proposed joint parameter and state estimation analysis of tracer test data proves very useful to obtain parameter estimates and their associated uncertainty for predictive modeling of radionuclide transport at the larger spatial scale.

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