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Stochastic conditional inverse modeling of subsurface mass transport: A brief review and the self-calibrating method

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Abstract. Conditioning transmissivity realizations to state variable data is complex due to the non-linear dependence of transmissivity (or any univariate transform of it) and piezometric heads, concentrations or velocities. A review of the literature shows these complexities. The self-calibrating algorithm combines standard geostatistics and non-linear optimization in a way that allows the generation of multiple realizations of logtransmissivity, which are conditioned not only to logtransmissivity measurements but also to piezometric head and concentration data. The self-calibrating method is demonstrated in a two-dimensional synthetic exercise in which the trade-offs between transmissivity, piezometric head and concentration data are analyzed.

Keywords: Stochastic inverse modeling, Worth of data, Inverse conditional realizations, Geostatistics, Non-linear optimization, Uncertainty, Monte-Carlo analysis

Introduction

Notwithstanding the very important, and almost always disregarded, problem of conceptual model uncertainty, the reliability of groundwater flow and mass transport in the subsurface depends very much on the characterization of the spatial variability of the parameters controlling the two state equations: the diffusion equation for flow and the advection-dispersion equation for transport, which in 2D, for vertically averaged quantities are:

$$\nabla \cdot (\mathbf{T} \cdot \nabla h) = S\frac{\partial h}{\partial t} + W \tag{1}$$

$$\nabla \cdot (\phi \mathbf{D} \cdot \nabla c - \phi \mathbf{v} c) = \phi \frac{\partial c}{\partial t} + q \tag{2}$$

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where **T** is the transmissivity tensor, S is storage coefficient, W represents external actions (extractions or recharges), ϕ is porosity, q represents sinks or sources of solute; h is piezometric head, and c is concentration; **D** is the hydrodynamic dispersion tensor, which depends on dispersivities and velocities, and **v** is the pore velocity vector (**D** and **v** couple the two equations), and finally, t is time. The partial derivatives with respect to the space coordinates (**u**) are embedded in the gradient (∇) and divergence ($\nabla\cdot$) operators.

These two equations with appropriate boundary and initial conditions provide the state of the system, which is given by $h(\mathbf{u}, t)$ and $c(\mathbf{u}, t)$. All parameters intervening in the equation could be spatially and/or temporally variable. Of all of them, we will focus on the spatially varying transmissivity.

Parameters and state variables are only known at a few locations; however, the state equation relates parameters and state variables over the entire domain of interest. If parameter values and external actions were known deterministically over the entire aquifer domain, we could obtain a deterministic description of the state of the system. In such a case, and barring conceptual model uncertainty, the reliability of the model would depend exclusively in the approximations taken to solve, analytically or numerically, the partial differential equations.

Unfortunately, parameter values display a large spatial variability that makes them impossible to predict at unsampled locations without uncertainty. Therefore, improving the characterization of the spatial variability of the parameters will render more reliable models. The steps to build a reliable model would commence by: (i) characterizing statistically the spatial variability of the parameter, e.g., transmissivity; this implies to compute statistics such as mean, variance or spatial correlation functions, and (ii) collecting whatever data about the parameter there are, which should include both direct measurements (i.e., from boreholes, well tests) and indirect data (i.e., from geology, geophysics). Neither the statistical constraints nor the data collected are enough to determine unequivocally the parameter values at each location in space: there are many alternative equally likely representations that would be consistent with this information. The next step towards a reliable model is to collect data about the state variables (i.e., piezometric heads, solute concentrations) and use them, through some type of inverse procedure, to condition the parameter spatial variability. Each datum, of any kind, is a constraint to be met by the parameter spatial distribution; as the number of conditioning data increases, the alternative realizations of parameters are more alike, and thus, the model is more reliable.

The paper is an extension of the paper by Gómez-Hernández et al. (2003), it contains a brief, non-exhaustive literature review on inverse modeling of transport, leading to the extension of the self-calibrating method (Sahuquillo et al., 1992; Gómez-Hernández et al., 1997; Capilla et al., 1997). The paper ends with an example demonstrating how incorporating aquifer state information about piezometric heads and concentrations improves the characterization of the spatial variability of transmissivities.

Review on inverse modeling of transport

Propagating and updating ensemble moments

One of the first works on inverse transport modeling is by Graham and McLaughlin (1989a, b). In their first paper, they derive the non-conditional moments of concentration for a given random function model of transmissivity and boundary and initial conditions. The stochastic equations in which (1) and (2) transform, once transmissivity is considered a space random function, are

used to obtain a linearized expression of velocity and concentration about their spatially variable expected values. This expression, which is valid for small variance of transmissivity, is then used to derive the cross-covariance between velocity and concentration, the velocity covariance and the concentration covariance. They finally obtain a set of coupled partial differential equations that describe the propagation in time of the first and second moments of velocities and concentrations. Although the solution for these moments provide information about uncertainties or the behavior of mean values, Graham and McLaughlin recognize that they are not useful in practice, since they are non-conditional, thus they cannot be applied to specific sites.

In their second paper, Graham and McLaughlin derive the conditional moment equations. A Kalman filter approach is used together with the propagation equations derived for the non-conditional moments, to update the first and second moments at each time step at which data are available. The updating was CPU-intensive, and it was decided that, assuming a weak correlation between concentrations and piezometric heads, the concentration moments could be made conditional to concentration data only, and the velocity moments could be made conditional to head and transmissivity data.

After testing the method on a synthetic study, they applied it to the simulation of chloride evolution at the Borden site. This was one of the first case studies in which concentration data are used together with transmissivity and hydraulic head data to calibrate the results of contaminant transport simulations. Half of the concentration measurements were used in the calibration and the other half for validation. The unconditional moment predictions show that peak concentration and spreading are predicted reasonably. However, there is significant uncertainty associated with these predictions. Conditioning to chloride concentrations results in the prediction of a more irregular plume, which fits better the observed values. The prediction uncertainty is smaller than in the non-conditional case, and the error predictions of the concentration measurements retained for validation is closer to zero.

The method presented by Graham and McLaughlin achieves its objectives and is capable of characterizing the conditional first and second moments (in space and time) of concentrations and fluid velocities. However, its application has not spread out. Some limitations of the method are: (i) the transmissivity field, which is the main source of uncertainty, is not updated as new measurements of hydraulic head and concentration are obtained; (ii) the method is limited to formations that are moderately heterogeneous in transmissivity, since it is based on a first-order perturbation approach; (iii) the method assumes that the random function model of transmissivity is multilognormal; (iv) the Kalman filter approach is very CPU-intensive, and (v) it is not clear how to account for uncertainties in the boundary conditions.

Semi-analytical Lagrangian approach

Rubin (1991a, b) formulates the conditioning of transport results on concentration measurements in a Lagrangian framework. In his first paper (Rubin, 1991a), he discusses how to condition on hydraulic head, transmissivity and velocity measurements. Similarly to Graham and McLaughlin (1989a, b), Rubin postulates a random space function model for transmissivity, which is multilognormal, stationary in mean and covariance, and with small variance. Then, he linearizes the groundwater flow equation for steady-state flow in an infinite domain without recharge to obtain linear expressions of hydraulic heads and velocities as a function of logtransmissivities. From the multinormality of logtransmissivity, it

follows that both hydraulic heads and concentrations are also multinormal, and therefore, the three variables, logtransmissivity, piezometric head and velocity, are jointly multinormal and fully characterized by their expected values and auto- and cross-covariances. These are derived taking advantage of the linearized expressions. Next, Rubin (1991a) proceeds to analyze advective transport from a continuous source by analyzing the trajectories followed by infinitesimal particles of solute mass. Due to the multinormality of velocities, it follows that particle trajectories can be characterized also by a multinormal distribution, characterized by a displacement mean, and a displacement covariance tensor. Finally, thanks to the congeniality of the multivariate multinormal distribution, it is immediate to extend all these expression to the conditional case, with measurements of transmissivity, piezometric head or velocity.

In his second paper, Rubin (1991b) extended the previous approach to incorporate concentration measurements. For a given discretization of the aquifer, the concentration of a given cell can be computed by adding up the mass carried out by the advected particles that are within the cell at a given time. By working with the one-particle trajectory probability distribution that can be obtained after tracking a sufficiently large number of particles on a conditional velocity field, and working with the two-particle trajectory probability distribution, which can be computed similarly, the concentration spatio-temporal covariances can also be computed. These covariances are then used in a cokriging formulation to get an estimate of the expected values of concentrations.

Some of the conclusions from the papers by Rubin are: (i) concentrations display a correlation function that is anisotropic, non-stationary and non-symmetrical, with a larger correlation between concentrations along the axis parallel to the flow direction than perpendicular to it; (ii) the correlation between concentrations at any two fix points in a Lagrangian co-ordinate system increases with time; (iii) the correlation between concentrations gets negative values before approaching zero for large distances; (iv) concentration variances are finite; (v) concentration data obtained at early time steps near the center of the plume are the most valuable for reducing prediction uncertainty.

The method discussed by Rubin (1991a, b) achieves its objective of determining conditional first and second moments of concentrations (in space and time), and has the same limitations as that of Graham and McLaughlin (1989a, b) except that it is much less computationally intensive, and therefore operative.

Maximum likelihood approach

The maximum likelihood approach was first introduced in the context of inverse modeling of groundwater flow by Carrera and Neuman (1986a, b, c) and it was extended to the inverse modeling of transport by Medina and others (Medina et al., 1990; Medina, 1993; Medina and Carrera, 1996). Although this method also aims at determining an "optimal" estimate of the spatial distribution of concentrations, and possibly an uncertainty estimate (similar to the conditional expectation and conditional covariance, respectively, of the methods described previously), the two most important advantages of this method are that during the inverse procedure the initial estimates of the parameters that control flow and transport are updated, especially transmissivities; and that the state equations (1) and (2) are used, for given initial and boundary conditions, without resorting to any linearization. Thus, the method recognizes that knowledge of the state of the system can improve our initial understanding of the spatial patterns of transmissivity, and it is not limited to moderately heterogeneous transmissivity fields.

The steps in the maximum likelihood approach applied to inverse transport modeling as described by Medina (1993) are the following: (i) the aquifer is discretized by finite elements, and initial estimates of the flow and transport parameters are made; these estimates are constant by user-defined zones in order to limit the number of parameter values that have to be estimated during the inversion procedure, and make the process stable; (ii) the groundwater flow and mass transport equations are solved numerically; (iii) an objective value is calculated with contributions from the mismatch between predicted and measured heads, from the mismatch between predicted and measured concentrations, and with the departure of the "optimal" estimates of the parameter values, such as transmissivities from their initial estimates; each one of these contributions is weighted by their covariance matrices; (iv) a minimization of the objective function is carried out by the Marquardt method, and the parameter values are updated. Steps (ii) to (iv) are repeated until the objective function is sufficiently small.

The maximum likelihood method is clearly superior to the two methods described previously for the reasons explained earlier. The two main drawbacks of the method in its original implementation are that the number of zones in which the aquifer is partitioned limits the degree of heterogeneity that can handle, and that uncertainty estimates are obtained through an estimation covariance which is derived after a linearization of the flow equation, thus is only approximate. It has been later recognized that alternative approaches to the parameterization of the heterogeneity of transmissivity can be accommodated by the maximum likelihood approach as powerful as those used by the self-calibrating approach described later.

An interesting application of the maximum likelihood method to the inverse modeling of transport can be found in the paper by Iribar et al. (1997). The authors state that this is the first calibration of a regional groundwater flow model with the help of both transient head data and concentration data. The problem addressed is that of seawater intrusion in the Llobregat delta aquifer, a few kilometers southwest of Barcelona, Spain. In this model, concentration data served to modify the conceptualization of the aquifer. The final model identified some zones of high transmissivity, corresponding to paleochannels, which were consistent with the geology of the site; the model was able to explain some features of the spatial distribution of chloride that could not be explained by previous models.

Sonnenborg et al. (1996) use a modified version of the maximum likelihood approach to invert not only for the parameters of the flow and transport equations, but also for the estimation of the mass release from the contamination source.

Mayer and Huang (1999) use a smooth estimate of transmissivity obtained by kriging as initial estimate for the spatial distribution of transmissivities, instead of an estimate by zones, and aimed to calibrate the values of the variogram parameters, instead of the parameter values directly.

The self-calibrating approach

All methods described above do not aim at the generation of multiple equally likely realizations of transmissivity fields conditional to transmissivity, piezometric head and concentration data. Instead, they seek estimates of transmissivities, piezometric heads and concentrations in some "optimal" sense; along with a covariance estimate for their uncertainty. The self-calibrating approach (Sahuquillo et al., 1992; Gómez-Hernández et al., 1997; Capilla et al., 1997, 1998)

was the first method developed with the aim of generating transmissivity realizations conditional to piezometric head data. It was extended for the conditioning to concentration data by Sahuquillo et al. (1999) and fully developed in the doctoral thesis of Hendricks Franssen (2001).

In the self-calibrating approach, multiple realizations of transmissivity are generated conditioned to both transmissivity data and state variable information. The process is sequential: first, a realization is generated conditioned only to transmissivity data, then this initial guess, or seed field, is modified through an optimization procedure until the state variable data is reproduced by the solution of the flow and transport equations in the updated field. Generating the seed field is simple using any of the available geostatistical techniques for conditional simulation of random fields. The key aspect of the method is the updating of the guess field in a way that does not destroy the conditioning to transmissivity data and maintains realistic patterns of spatial variability. The details of how the perturbation is computed are discribed next.

Let $\{\mathbf{T}\} = \{T_i,\ i = 1,...,N\}$ represent a realization of transmissivity over the N numerical cells discretizing the volume of study. This realization is conditional, by construction, to (n_T) data values, represented by $\{T_m\} = \{T_{im},\ i \in (n_T)\}$. Let $\{h\} = \{h_i,\ i = 1,...,N\}$, and $\{c\} = \{c_i,\ i = 1,...,N\}$, be the numerical solution of the groundwater flow and mass transport equations on this realization, $\{h_m\} = \{h_{im},\ i \in (n_h)\}$, be the set of (n_h) head measurements, and $\{c_m\} = \{c_{im},\ i \in (n_c)\}$, be the set of (n_c) concentration measurements to which we wish to condition $\{\mathbf{T}\}$. The penalty function $F = \sum_{i\in(nh)}(h_i - h_{im})^2 + \alpha \sum_{i\in(nc)}(c_i - c_{im})^2$ will not, in principle, be close to zero, indicating that measured heads and measured concentrations are not reproduced by the flow and transport simulations in the given transmissivity field. In such case, a perturbation $\{\Delta\mathbf{T}\} = \{\Delta T_i,\ i = 1,...,N\}$ is added to $\{\mathbf{T}\}$ so that the head and concentration solution in the updated field $\{\mathbf{T} + \Delta\mathbf{T}\}$ results in a penalty function close to zero. The perturbation $\{\Delta\mathbf{T}\}$ is parameterized as a linear function of the perturbations at a few selected master locations (m) uniformly distributed over the volume of interest. A rule of thumb to select the master locations is to have 1 or 2 master locations per correlation length. The perturbation at any cell i is given by

$$\delta T_i = \sum_{j\in(m)} \lambda_j \delta T_j$$

with λ_j computed by ordinary kriging with the same variogram used for the generation of $\{\mathbf{T}\}$. To ensure that conditioning to transmissivity is not destroyed by the perturbation, the set of master locations includes the transmissivity data locations, i.e., $(m) \supset (n_T)$ and the perturbation at the transmissivity data locations is set constant to zero, $\Delta T_i = 0,\ i \in (n_T)$. A non-linear optimization procedure determines the perturbations $\Delta T_i,\ i \in (m)$ that reduces the penalty function F, close to zero.

Including concentration data in the conditioning process is, from a formal point of view, identical to how piezometric data are included in the self-calibrating approach as described by Gómez-Hernández et al. (1997). However, from a practical point of view, it has represented a very importance challenge due to the complexity of the problem: the non-linear optimization step, which requires computing the sensitivity of the objective function to changes of transmissivity at the master locations is cumbersome and specific algorithms for this

Table 1. List of scenarios

Conditioning	20 Y data	20 h data	13 c data
Scenario 1	NO	NO	NO
Scenario 2	YES	NO	NO
Scenario 3	NO	YES	NO
Scenario 4	YES	YES	NO
Scenario 5	NO	NO	YES
Scenario 6	YES	NO	YES
Scenario 7	NO	YES	YES
Scenario 8	YES	YES	YES

purpose had to be developed. The reader interested in the specifics of the self-calibrating approach for concentration conditioning is referred to Sahuquillo et al. (1999) and, especially, to Hendricks Franssen (2001).

Example application

The extended self-calibrating algorithm has been applied under controlled conditions to a synthetic aquifer. In the synthetic aquifer, the exact response to flow and transport of the aquifer is known. The aquifer of 500 m by 500 m extent is discretized into 50 by 50 cells, with heterogeneous log-transmissivities of mean −6 ($\log_{10}$ m^2/s), standard deviation of 0.5 ($\log_{10}$ m^2/s), and isotropic variogram with range of 125 m. The flow regime is at steady state with a linear average head gradient. A contamination event was simulated resembling a spill over a rectangular area of 10 m by 100 m near one of the edges of the aquifer. The numerical solution of the groundwater flow and mass transport equations was obtained; then, the fields were sampled for a few data values of the parameters and the state variables, more precisely 20 log transmissivity data (Y), 20 piezometric head data (h) and 13 concentration data (c) at a time step in which half of the plume had already past the concentration control locations. The scenarios described in Table 1 were considered as with regard to conditioning data combinations.

For each scenario, 100 realizations conditioned to the corresponding combination of data were generated. The resulting ensemble of realizations is a stochastic conditional model of the aquifer. The reliability of the model was analyzed by measuring the average departure, at each of the 2500-discretization cells between the average of the 100 realizations and the reference fields (AAE(·)), and the average local standard deviation of the 100 realizations (AASD(·)):

$$\mathrm{AAE}(X) = \frac{1}{\mathrm{NNODES}} \sum_{i=1}^{\mathrm{NNODES}} \left(\overline{X}_{\mathrm{SIM},i} - X_{\mathrm{REF},i}\right)$$

$$\mathrm{AESD}(X) = \frac{1}{\mathrm{NNODES}} \sum_{i=1}^{\mathrm{NNODES}} \sigma_{X_i}$$

where AAE is average absolute error, AESD average ensemble standard deviation, NNODES the number of discretization grid cells, and i is a grid cell index, X represents either decimal log transmissivity, steady-state hydraulic head or mass concentration at a certain time step, the overbar indicates ensemble

average, the subscript SIM refers to the realizations, and the subscript REF to the reference values; finally, σ_{Xi} is the ensemble standard deviation of X at a given node. The average absolute error measures how closely, on average, the ensemble mean of the 100 realizations predicts the reference field, and the average standard deviation measures how much uncertainty there is about the ensemble mean, the combination of both values is a good measure of the reliability of the model.

Tables 2 and 3 show the average values AAE and AESD for the different scenarios and for log-transmissivity, piezometric head and concentration. For comparison purposes, all values have been standardized with respect to the unconditional scenario, thus allowing easy comparison of the relative gain that introducing a given combination of conditioning data brings.

The tables indicate clearly how the use of conditioning data improves both the average absolute error and the average standard deviation. With the exception of scenario number 5, for which only concentration data is used, and for which the average standard deviation is larger than for the unconditional case, (although the predictions improve, they are more uncertain) the influence that the different data types have in the characterization/prediction of transmissivity and piezometric head and concentration is noticeable (and expectable). When each data type is used alone, the best prediction occurs for that specific variable, and when different data types are used, their combined effect multiplies the reliability of the model.

Table 2. Standardized average absolute error (scenario 1 = 100) for the characterization of the transmissivity, steady-state head, and concentration (averaged over 20 time steps) fields. (The letter *Y* or *N* indicates whether the data type was used for conditioning.)

	AAE(Y)	AAE(h)	AAE(c)
Scenario 1	100 *N*	100 *N*	100 *N*
Scenario 2	92 *Y*	93 *N*	68 *N*
Scenario 3	91 *N*	49 *Y*	97 *N*
Scenario 4	81 *Y*	34 *Y*	70 *Y*
Scenario 5	96 *N*	92 *N*	54 *Y*
Scenario 6	91 *Y*	90 *N*	58 *Y*
Scenario 7	88 *N*	52 *Y*	43 *Y*
Scenario 8	79 *Y*	35 *Y*	37 *Y*

Table 3. Standardized average ensemble standard deviation (scenario 1 = 100) for the characterization of the transmissivity, steady-state head and, concentration (averaged over 20 time steps) fields. (The letter *Y* or *N* indicates whether the data type was used for conditioning.)

	AESD(Y)	AESD(h)	AESD(c)
Scenario 1	100 *N*	100 *N*	100 *N*
Scenario 2	85 *Y*	79 *N*	95 *N*
Scenario 3	96 *N*	59 *Y*	97 *N*
Scenario 4	81 *Y*	51 *Y*	82 *N*
Scenario 5	107 *N*	105 *N*	108 *Y*
Scenario 6	88 *Y*	82 *N*	90 *Y*
Scenario 7	98 *N*	61 *Y*	84 *Y*
Scenario 8	81 *Y*	50 *Y*	69 *Y*

Conclusions

The self-calibrating algorithm for conditioning transmissivity realizations is a valuable tool for building ensembles of realizations conditioned to different data types. Post-processing of these ensembles of realizations provide different model reliability measures. In the 2-D synthetic example discussed here, the existence of a reference field permits evaluating prediction bias (average departure between realizations and reference) besides uncertainty (average local standard deviation).

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