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Computational aspects of the coupled inversion of groundwater flow and mass transport

A. SAHUQUILLO, H. J. W. M. HENDRICKS FRANSSEN, J. J. GÓMEZ-HERNÁNDEZ

Departamento de Ingeniería Hidráulica y Medio Ambiente, Universidad Politécnica de Valencia, C. Camino de Vera s/n, E-46011 Valencia, Spain

e-mail: harrie@dihma.upv.es

J. E. CAPILLA

Departamento de Física Aplicada, Universidad Politécnica de Valencia, C. Camino de Vera s/n, E-46011 Valencia, Spain

Abstract The sequential self-calibrated method has been extended to the coupled stochastic inverse modelling of transient groundwater flow and contaminant mass transport. The paper focuses on the calculation of the gradient vector, which contains the partial derivatives of the objective function with respect to perturbation parameters like transmissivities, prescribed head values, retardation factors and mass release information.

INTRODUCTION

Our objective is to simulate multiple equally likely solutions to the coupled three-dimensional (3-D) groundwater flow and contaminant mass transport inverse problem. The sequential self calibrated method (Sahuquillo *et al.*, 1992; Gómez-Hernández *et al.*, 1997; Capilla *et al.*, 1997), originally formulated for two-dimensional (2-D) steady state groundwater flow, was recently extended to transient flow (Hendricks Franssen *et al.*, 1999a) and 3-D flow in fractured media (Hendricks Franssen *et al.*, 1999b). The method was tested in both synthetic studies and case studies. In this paper an extension for conditioning to concentration measurements is presented. Concentration data contain important information on the groundwater flow field and therefore it is expected that conditioning to these data improves the characterization of the spatial variable transmissivities and possibly other parameters. We discuss the equations for the 2-D case in order to avoid long formulations.

FLOW AND TRANSPORT EQUATIONS

As in the inverse modelling of groundwater flow, a geostatistical simulation algorithm is used to generate a series of transmissivity realizations conditional to transmissivity data. Each of these transmissivity realizations is used, together with boundary conditions, specified recharges and discharges, initial conditions, storativity coefficients, dispersivity values and contaminant release information, to obtain a solution of the groundwater flow and the mass transport equations.

The groundwater flow equation is formulated as follows:

$$\frac{\partial}{\partial x}\left(T(x,y)\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T(x,y)\frac{\partial h}{\partial y}\right)+w(x,y,t)=S(x,y)\frac{\partial h}{\partial t} \tag{1}$$

in which x and y are the spatial co-ordinates [L], t is time [T], h is hydraulic head [L], T is transmissivity [$L^2 T^{-1}$], w are sources (+) and sinks (–) [$L\,T^{-1}$] and S is the storativity coefficient [–]. The groundwater flow equation is solved by finite differences resulting in the following linear system of equations:

$$[\mathbf{A}]\{\mathbf{h}\}+\{\mathbf{W}\}=[\mathbf{SF}]\frac{\partial\{\mathbf{h}\}}{\partial t} \tag{2}$$

where [**A**] is the conductance matrix, {**h**} the vector containing unknown head values, {**W**} the vector with sinks and sources, probably variable in time and [**SF**] the storage matrix.

The mass transport equation is formulated as follows:

$$\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x}+D_{xy}\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c}{\partial x}+D_{yy}\frac{\partial c}{\partial y}\right)-\frac{\partial}{\partial x}(q_x c)-\frac{\partial}{\partial y}(q_y c)+\frac{wc''}{b}-\lambda R\phi c = \phi R\frac{\partial c}{\partial t} \tag{3}$$

in which c is concentration [$M\,L^{-3}$], q_x and q_y components of the Darcy velocity vector **q** [$L\,T^{-1}$], w injection rate [$L\,T^{-1}$], c mass concentration of the water injected, b aquifer depth [L], λ decay rate [T^{-1}], R retardation factor [–], ϕ porosity [–]. D_{xx}, D_{xy}, D_{yx} and D_{yy} are components of the dispersion tensor **D** [$L^2 T^{-1}$]:

$$D_{xx}=\alpha_L\frac{q_x^2}{|\mathbf{q}|}+\alpha_T\frac{q_y^2}{|\mathbf{q}|}\quad D_{yy}=\alpha_T\frac{q_x^2}{|\mathbf{q}|}+\alpha_L\frac{q_y^2}{|\mathbf{q}|}\quad D_{xy}=D_{yx}=(\alpha_L-\alpha_T)\frac{q_x q_y}{|\mathbf{q}|} \tag{4}$$

in which α_L is the longitudinal dispersivity coefficient [L], α_T the transversal dispersivity coefficient [L] and [**q**] the norm of vector **q**.

The components of the dispersivity tensor depend on the groundwater flow velocities, which are obtained by solving the groundwater flow equation. Finite differences formulation of equation (3), using bilinear interpolation for the flux vector components, results in the following discretized version of the transport equation:

$$D^{EA}c_A+D^{EB}c_B+D^{EC}c_C+D^{ED}c_D+D^{EE}c_E+D^{EF}c_F+D^{EG}c_G+D^{EH}c_H+D^{EI}c_I + Z_E = E_E\frac{\partial c}{\partial t} \tag{5}$$

in which the superscripts refer to cells according to Fig. 1. Some of the values of the coefficients from equation (5) are given below (the expressions for the rest of the coefficients are similar):

$$D^{EA}=\frac{1}{4}(D_{xy,ED}+D_{xy,EB}) \tag{6}$$

$$D^{EB} = \frac{1}{4}(D_{xy,ED} - D_{xy,EF}) + \frac{\Delta x}{\Delta y} D_{yy,EB} + \frac{\Delta x}{2} q_{y,EB}$$

$$D^{EE} = -\frac{\Delta y}{\Delta x}(D_{xx,EF} - D_{xx,ED}) - \frac{\Delta x}{\Delta y}(D_{yy,EH} + D_{yy,EB}) + \frac{\Delta y}{2}\left(q_{x,ED} - q_{x,EF}\right) +$$
$$\frac{\Delta x}{2}\left(q_{y,EB} - q_{y,EH}\right) - \lambda \phi R \Delta x \Delta y$$

$$Z_E = \frac{c'' w}{b} \Delta x \Delta y$$

$$E_E = \Delta x \Delta y \phi R$$

in which Δx and Δy are the cell size [L] along the x-axis and the y-axis, respectively. The double superscripts indicate that the parameter has to be evaluated at the cell interface. Equation (5) can be written in matricial form:

$$[\mathbf{D}]\{\mathbf{c}\} + \{\mathbf{Z}\} = [\mathbf{E}]\frac{\partial \{\mathbf{c}\}}{\partial t} \tag{7}$$

In order to evaluate the reproduction of the measured heads and concentration values by the simulated ones, an objective function is formulated as follows:

$$F = \sum_i \int_0^t [\mathbf{W}_h]\{\mathbf{h}_i - \mathbf{h}_i^*\}^2 \mathrm{d}t + \psi_1 \sum_i \int_0^t [\mathbf{W}_c]\{\mathbf{c}_i - \mathbf{c}_i^*\}^2 \mathrm{d}t + \psi_2 \sum_i \mathbf{W}_k (P_i - P_i^*)^2 \tag{8}$$

in which t is time, h_i are time dependent head values, c_i are time dependent concentration values, P_i are parameter values, $\mathbf{W}_h$, $\mathbf{W}_c$ and $\mathbf{W}_k$ are weighting matrices and ψ_1 and ψ_2 are trade-off coefficients. The asterisk denotes measurements and the summations extend to the respective measurement locations (not necessarily the same for all variables).

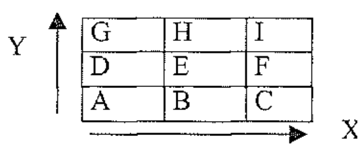

Fig. 1 Nodes in a finite difference scheme.

THE SELF-CALIBRATION PROCESS

If F is larger than a user-defined value an additional conditioning step starts in order to reproduce the measured hydraulic head and concentration values. In an iterative approach, in which the groundwater flow and mass transport equation are solved numerous times, a transmissivity perturbation field ΔY is determined by a combination of nonlinear optimization and geostatistics, so that the sum of the starting field plus the perturbation yields a transmissivity field in which the solution of the groundwater flow and mass transport equation match the measured head and concentration data. Other variables could be jointly calibrated with the transmissivities using a similar procedure, such as storativities (Hendricks Franssen *et al.*, 1999a), or recharges.

The perturbation parameters are the transmissivities (and the other parameters subject to calibration, if any) at selected master blocks which form a small subset of the grid cells. Master blocks are used in order to reduce the dimensions of the vectors and matrices of equations (14)–(16) (see below). The perturbations at the remaining grid cells are obtained by ordinary kriging interpolation of the master block perturbations. The perturbations are optimized at the selected master blocks by calculating the gradient of the objective function with respect to the perturbation parameters and using nonlinear optimization algorithms to calculate an updating direction. Now we will focus on the computational aspects of the calculation of the gradient.

The optimization procedure we propose is related to the work of Carrera & Medina (1994) with some modifications which we think are advantageous. The conditioning to concentration measurements is very CPU intensive and the most CPU consuming step is the calculation of the gradient of the objective function with respect to the perturbation parameters (transmissivities and possibly other parameters). We have formulated the conditioning in an Eulerian framework with the help of adjoint state equations. The adjoint state formulation is advantageous; for the calibration of heads the required CPU time is reduced because the Jacobian does not have to be calculated. However, later it will be seen that if the calibration of concentrations is included the Jacobian containing the derivatives of heads with respect to perturbation parameters has to be computed in this proposed formulation. Therefore, it could be decided to apply the adjoint state formulation only to the transport equation and obtain the derivatives of the flow equation with respect to the perturbation parameters directly. A major difference from other existing formulations is that the temporal domain is not discretized. The state equations of the discretized domain are formulated as follows:

$$\Psi = [\mathbf{A}]\{\mathbf{h}\} + \{\mathbf{W}\} - [\mathbf{SF}]\frac{\partial\{\mathbf{h}\}}{\partial t} = 0 \tag{9}$$

$$\Theta = [\mathbf{D}]\{\mathbf{c}\} + \{\mathbf{Z}\} - [\mathbf{E}]\frac{\partial\{\mathbf{c}\}}{\partial t} = 0 \tag{10}$$

with Ψ and Θ being the states of the groundwater flow and mass transport equation respectively. The Lagrangian is:

$$\Im = F + \int_0^t \{\nu\}^T\{\Psi\}\mathrm{d}t + \int_0^t \{\mu\}^T\{\Theta\}\mathrm{d}t \tag{11}$$

with $\{\nu\}$ and $\{\mu\}$ being Lagrange multipliers, also called adjoint states, which are time dependent. The Lagrangian multipliers are found by solving equations (12) and (13) which are identical to the steady groundwater flow and the mass transport equation:

$$2\{\mathbf{W}_h(\mathbf{h} - \mathbf{h}^*)\}^T + \{\nu\}^T[\mathbf{A}] = 0 \tag{12}$$

$$2\{\mathbf{W}_c(\mathbf{c} - \mathbf{c}^*)\}^T + \{\mu\}^T[\mathbf{D}] = 0 \tag{13}$$

Equations (12) and (13) only have to be solved for the time steps at which measurements are available, and not for all time steps at which the groundwater flow and mass transport equation are solved, as would be the case if the state equations were discretized in time. Taking derivatives of the Lagrangian with respect to the perturbation parameters P_k yields:

$$\frac{\partial \Im}{\partial P_k} = \frac{\partial F}{\partial P_k} + \int_0^t \{\nu\}^T \left\{\frac{\partial \Psi}{\partial \mathbf{P}_k}\right\} \mathrm{d}t + \int_0^t \{\mu\}^T \left\{\frac{\partial \Theta}{\partial \mathbf{P}_k}\right\} \mathrm{d}t \tag{14}$$

The Lagrangian multipliers are found by applying (12) and (13) and the derivatives of the states with respect to the perturbation parameters are given by:

$$\left\{\frac{\partial \Psi}{\partial \mathbf{P}_k}\right\} = \left[\frac{\partial \mathbf{A}}{\partial \mathbf{P}_k}\right]\{\mathbf{h}\} + \left\{\frac{\partial \mathbf{W}}{\partial \mathbf{P}_k}\right\} - \left[\frac{\partial \mathbf{SF}}{\partial \mathbf{P}_k}\right]\left\{\frac{\partial \mathbf{h}}{\partial t}\right\} \tag{15}$$

$$\left\{\frac{\partial \Theta}{\partial \mathbf{P}_k}\right\} = \left[\frac{\partial \mathbf{D}}{\partial \mathbf{P}_k}\right]\{\mathbf{c}\} + \left\{\frac{\partial \mathbf{Z}}{\partial \mathbf{P}_k}\right\} - \left[\frac{\partial \mathbf{E}}{\partial \mathbf{P}_k}\right]\left\{\frac{\partial \mathbf{c}}{\partial t}\right\} \tag{16}$$

The partial derivatives in the equation (15) are given by Gómez-Hernández *et al.* (1997). In these expressions, kriging coefficients appear due to the fact that the perturbations at the master blocks are interpolated by kriging to the rest of the grid cells.

The most time consuming partial derivatives to calculate in equation (16) are $\partial \mathbf{D}/\partial \mathbf{P}_k$. The derivatives of the fluxes with respect to the perturbation parameters have to be calculated (see also equations (4) and (6)). The components of the flux vector for the fluxes between for example the cells E and F are given by:

$$q_x^{EF} = -T_{EF}\frac{h_F - h_E}{\Delta x} \qquad q_y^{EF} = -T_E\frac{h_H - h_B}{4\Delta y} - T_F\frac{h_I - h_C}{4\Delta y} \tag{17}$$

The derivatives of these flux components with respect to perturbation of decimal log transmissivity ΔY_k at the master location are given then by:

$$\frac{\partial q_{x,EF}}{\partial \Delta Y_k} = \frac{1}{2}\left(\lambda_E^k + \lambda_F^k\right) q_{x,EF} + \frac{T_{EF}}{\Delta x}\left(\frac{\partial h_F}{\partial \Delta Y_k} - \frac{\partial h_E}{\partial \Delta Y_k}\right) \tag{18}$$

$$\begin{aligned}\frac{\partial q_{y,EF}}{\partial \Delta Y_k} = &-\lambda_E^k T_E\frac{h_H - h_B}{4\Delta y} - \lambda_F^k T_F\frac{h_I - h_C}{4\Delta y} - \frac{T_E}{4\Delta y}\left(\frac{\partial h_H}{\partial \Delta Y_k} - \frac{\partial h_B}{\partial \Delta Y_k}\right)\\ &- \frac{T_F}{4\Delta y}\left(\frac{\partial h_I}{\partial \Delta Y_k} - \frac{\partial h_C}{\partial \Delta Y_k}\right)\end{aligned} \tag{19}$$

where λ_E^k is the kriging weight applied to the master block perturbation for the interpolation of the perturbation at cell E. We only consider the derivatives $\partial \mathbf{D}/\partial \Delta Y_k$ related to convective transport, in order to avoid cumbersome calculations. This simplification should have a minor impact on the calculation of the objective function gradient when convective transport dominates dispersive transport. Equations (18) and (19) require calculation of the Jacobian of heads. This can be obtained by solving the sensitivity equations resulting after taking derivatives of the flow equation and rearranging:

$$A\frac{\partial h}{\partial \Delta Y_k}+\left[\frac{\partial A}{\partial \Delta Y_k}h+\frac{\partial W}{\partial \Delta Y_k}-\frac{\partial SF}{\partial \Delta Y_k}\frac{\partial h}{\partial t}\right]=\mathbf{SF}\frac{\partial h/\partial \Delta Y_k}{\partial t} \tag{20}$$

Equation (20) has the same format as the flow equation, the head derivative with respect to the transmissivity perturbation being the unknown vector.

Other derivatives which appear in equation (16) with respect to the perturbation of transmissivity are zero. Partial derivatives with respect to the perturbation of other parameters can be obtained in a similar way. The only non zero derivatives with respect to the perturbation of prescribed head boundaries (Δh_k^{Γ}) are the derivatives of the elements of **D** (not given here). Furthermore, derivatives with respect to the perturbation of storativities and recharges have also been obtained.

Also the parameters involved in the transport equation may be subject to calibration. Derivatives with respect to the perturbation of the dispersivity coefficients (equation (4)) can be obtained easily, but we consider that the perturbation of the dispersivity coefficients is irrelevant because the spatial variability of transmissivity accounts for most of the dispersive part of the groundwater flow. Furthermore, the conceptual significance of the dispersivity coefficients is unclear. Other relevant parameters that can be perturbed are the retardation coefficient and the mass release. Spatial variability on the retardation coefficient can be easily accounted for, using a similar approach for the spatially variable retardation coefficients as for the spatial variable transmissivity and storativity fields. However, the main practical problem with the calibration of spatially variable retardation coefficients is that very few measurements are available, so that it is difficult to make reliable prior estimations. The calibration of mass release is as difficult as that of retardation coefficients, although sometimes more or less precise estimates of the mass release can be made.

DISCUSSION AND CONCLUSIONS

The approach presented for the stochastic inverse modelling of groundwater flow and mass transport results in a series of equally likely solutions to the coupled flow and transport problem. The reproduction of not only head measurement data, but also concentration data, is expected to reduce the ensemble variance and result in an ensemble average more close to "reality", because the individual simulations are more data charged. In order to achieve the conditioning to concentration data, the gradient of the objective function with respect to the perturbation parameters has to be calculated. The adjoint state approach is used in this article to calculate the gradient. The adjoint state equations are formulated continuously in time so that the equations only have to be solved for those time steps at which measurement data are available. Some of the partial derivatives of the matrices with respect to the perturbation parameters are given in the article.

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