A NEWTON-RAPHSON BASED CODE FOR SEAWATER INTRUSION MODELLING AND PARAMETER ESTIMATION

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Abstract

A new code called TRANSDENS for simulation and parameter estimation in density-dependent flow and solute transport is presented. Flow and transport are solved in terms of fresh water head and solute mass fraction respectively. The code allows solving the coupled problem using Picard iterations, the Newton-Raphson method or a combination of both to improve convergence. Also, different ways of matrix storage are available, and both an iterative and a direct solver for the final linear system of equations are available. The inversion of parameters is based on the maximum likelihood method. It takes advantage of the previously calculated Jacobian matrix in Newton-Raphson method during the direct problem solution as described by Slooten *et al.* (2002). The Henry problem, a usual benchmark for saltwater intrusion codes, is used for code validation.

Keywords: salt water intrusion, parameter estimation, numerical modelling, variable density.

Introduction

Variable density and viscosity fluids are common in hydrogeology. A change of fluid properties may have significant consequences on the behaviour of the hydrological systems and it is sometimes of vital importance to accurately describe the aquifer dynamics. Both density and viscosity are dependent on temperature, solute concentration and pressure. However, density of groundwater is mainly affected by solute concentration while viscosity is by temperature. Changes in the density of groundwater can appear for example in coastal aquifers due to saltwater intrusion, or in salt bearing aquifers due to mineral dissolution. Viscosity variations can be found in geothermal aquifers or in the surroundings of nuclear repositories test sites where the aquifer is heated artificially. Sometimes both effects are present, such as

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in the case of brines, where the high concentrations of salt make density and viscosity variations important. They may also appear in arid areas where a big gradient of temperature through the unsaturated zone exists and evaporation increments water salinity.

Density dependent flow is a well-known phenomenon. From the work of Bear (1972) to the most recent reviews by Kolditz *et al*. (1998), Holzbecher (1998) and Diersch and Kolditz (2002) it has been fully described.

Under variable density or viscosity conditions, flow and transport equations form a coupled non-linear phenomenon. Simulation, then, requires an iterative approach that can be subject to convergence problems and be highly computationally demanding. Many codes are available for the simulation of density dependent flow and transport. Among others, SUTRA (Voss, 1984), HYDRUS-2D (Simunek *et al*., 1998), ROCKFLOW (Kolditz *et al*., 1999), MOCDENSE (Sandford and Konikow, 1985), MOCDENS3D (Oude Essink, 1998) SALTFLOW (Molson and Frind, 1994) and SEAWAT (Guo and Langevin, 1998) can be mentioned. All of them use an iterative scheme known as the Picard scheme (see next section) to solve the coupling between flow and transport equations. However, when applying calibration techniques (none of the above codes use automatic calibration procedures), it is even more important that the chosen algorithm is both fast and robust. Newton-Raphson based algorithms are therefore a feasible alternative which has been implemented by codes such as CODE_BRIGHT (Olivella *et al*., 1996), FEFLOW (Diersch, 2002) or d3f (Fein and Schneider, 1998) for density-dependent problems. Also Putti and Paniconi (1995) developed a partial Newton scheme (neglecting some of the off-diagonal terms in the Jacobian matrix) that proved to be more robust and efficient than Picard iterations.

Automatic calibration is not a usual point in variable density codes. However, in groundwater modelling one of the main sources of uncertainty is the value of the hydraulic parameters involved in the model (conductivity, storage, porosity, etc.). Their values are usually chosen according to field tests, geological characteristics of the aquifer and assorted previous information. To reduce their uncertainty, automatic calibration has proved to be a useful tool. The parameters are calculated such as the values that minimize a certain objective function that measures the difference between the computed and observed values of state variables. The obtained parameter values tend to be more reliable and robust than those obtained by manual calibration; furthermore the minimization methodology allows for a rough quantification of uncertainty in the parameters and the model predictions. Recent overviews of inverse methods in hydrogeology have been given by McLaughlin and Townley (1996), de Marsily *et al*. (2000) or Carrera *et al*. (in press).

Calibration techniques tend to be more robust when different types of state variables are used. In density dependent problems, it is natural to use both flow and transport data. The movement of the saltwater-freshwater interface for instance can be seen as an aquifer-scale tracer test that gives a huge amount of valuable information about the parameter fields. However, although automatic calibration has been often applied to hydrological models, there is little experience in automatic calibration of systems where density or viscosity variations play an important role.

The iterative nature of the calibration process becomes critical when density-dependent flow is present. Due to the non-linearity of flow and transport, two inner iteration loops are found in the calibration main

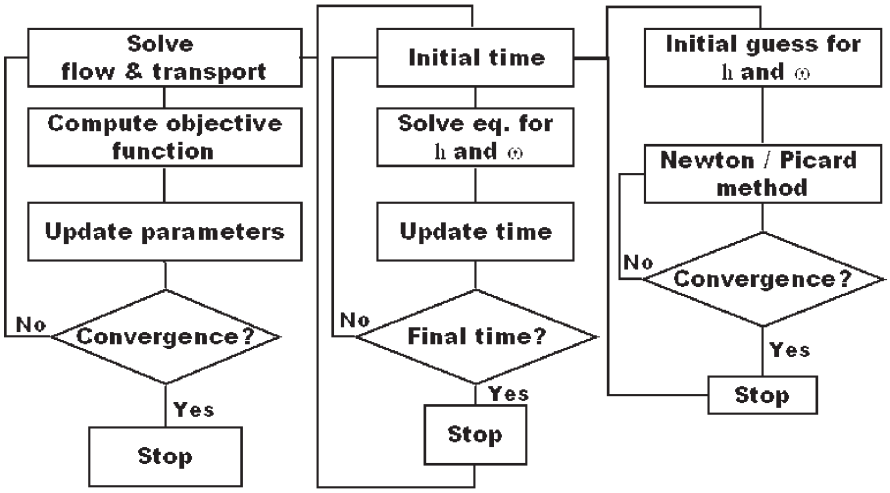

Figure 1. Automatic parameter calibration process showing the inner loops corresponding to the solution of the non-linear coupled flow and transport equations (h stands for equivalent fresh water head and w for solute mass fraction).

loop as shown in Figure 1. Since for every calibration iteration the whole simulation problem has to be solved, if simulation fails to converge, the whole calibration process fails. So it is of utmost importance to use a robust method and an efficient algorithm for solving the non-linear simulation problem. Also the computational demand can be highly increased. Therefore efficiency is also a must in the used algorithms.

A code for saltwater intrusion modeling and parameter estimation called TRANSDENS is presented. The code is based on a Newton-Raphson algorithm that aims maximum efficiency on the simulation process according to the former criteria.

Methodology

Governing equations

The flow equation is expressed in terms of equivalent freshwater head h_f. The equivalent freshwater head is defined as

$$h_f = \frac{P}{\rho_f g} + z \tag{1}$$

where P is fluid pressure, ρ_f is the density of the fresh water, g the module of gravity and z the elevation. It has to be remarked that elevation is in the opposite direction of gravity.

Density is considered only as a function of the transport state variable, ω, which can be either temperature (ºC) or solute mass fraction (kg of solute per kg of fluid). Density is approximated by

$$\rho = \rho_f e^{\beta_\omega (\omega - \omega_0)} \tag{2}$$

where ω_0 is the mass fraction of reference (at which $\rho = \rho_f$) and β_ω is defined as

$$\beta_\omega = \frac{1}{\rho}\frac{\partial \rho}{\partial \omega} \tag{3}$$

The value of β_ω and ρ_f can be changed in order to get a better description of the density. For seawater intrusion ρ_f can be taken as 1000 kg/m^3 and β_ω equal to 0.7.

The flow equation in terms of equivalent fresh water heads is

$$\frac{\partial \Theta}{\partial h_f}\frac{\partial h_f}{\partial t} + \Theta \beta_\omega \frac{\partial \omega}{\partial t} = -\frac{1}{\rho}\nabla\cdot[\rho \mathbf{q}] + \frac{\rho^*}{\rho} q_s \tag{4}$$

where Θ is the fluid content per volume of aquifer, q_r stands for sink and sources, ρ^* is the density of the sink/source fluid and **q** is Darcy's velocity

$$\frac{\partial \Theta}{\partial h_f}\frac{\partial h_f}{\partial t} + \Theta \beta_\omega \frac{\partial \omega}{\partial t} = -\frac{1}{\rho}\nabla\cdot[\rho \mathbf{q}] + \frac{\rho^*}{\rho} q_s \tag{5}$$

where μ and μ_f are fluid viscosity and reference viscosity respectively and **K** is hydraulic conductivity at ω_0 (what makes necessary to explicitly include the viscosity variations in the formula). For the range of concentrations involved in seawater intrusion, viscosity variations can be neglected (Bear, 1972).

Then transport equation is expressed in terms of solute mass fraction

$$[\Theta + \alpha_s]\frac{\partial \omega}{\partial t} = -\mathbf{q}\nabla\omega + \frac{1}{\rho}\nabla(\rho \mathbf{D}\nabla\omega) - \lambda[\Theta + \alpha_s]\omega + q_s\left(\frac{\rho^*}{\rho}\omega^* - \omega\right) \tag{6}$$

where α_s is the retardation coefficient, **D** is the diffusive-dispersive tensor, λ accounts for the first order decay processes and ω^* is the mass fraction of sink/source fluid.

Both equations (4) and (6) are divided by the density of the system. This does not affect the modelling of the phenomenon and was done for coding purposes.

Solution method

Flow and transport equations are coupled and non-linear under variable density conditions. Equations (4) and (6) are solved with the finite element method for the spatial discretization and a weighted finite differences method for the temporal discretization. This leads to a set of non-linear algebraic equations that can be solved either with Picard iterations or the Newton- Raphson method.

Picard Iterations

Picard's method solves flow and transport equations as if they were uncoupled. The solution of the flow equation is solved to compute the Darcy's velocity used in the transport equation. For the next iteration flow is solved using the previously computed mass fraction and the scheme is repeated until convergence.

Newton-Raphson's method

Newton-Raphson is also an iterative method. For each iteration, the increment of state variables is the solution of the following system of equations:

$$\begin{pmatrix} \frac{\partial \mathbf{f}_f}{\partial \mathbf{h}_f}(\mathbf{h}_f^k, \boldsymbol{\omega}^k) & \frac{\partial \mathbf{f}_f}{\partial \boldsymbol{\omega}}(\mathbf{h}_f^k, \boldsymbol{\omega}^k) \\ \frac{\partial \mathbf{f}_T}{\partial \mathbf{h}_f}(\mathbf{h}_f^k, \boldsymbol{\omega}^k) & \frac{\partial \mathbf{f}_T}{\partial \boldsymbol{\omega}}(\mathbf{h}_f^k, \boldsymbol{\omega}^k) \end{pmatrix} \begin{pmatrix} \Delta \mathbf{h}_f^k \\ \Delta \boldsymbol{\omega}^k \end{pmatrix} = - \begin{pmatrix} \mathbf{f}_f(\mathbf{h}_f^k, \boldsymbol{\omega}^k) \\ \mathbf{f}_T(\mathbf{h}_f^k, \boldsymbol{\omega}^k) \end{pmatrix} ; \quad \mathbf{h}_f^{k+1} = \mathbf{h}_f^k + \Delta \mathbf{h}_f^k ; \quad \boldsymbol{\omega}^{k+1} = \boldsymbol{\omega}^k + \Delta \boldsymbol{\omega} \tag{7}$$

Bold letters indicate vectors. The superscript k indicates the time step, $\mathbf{f}_f(\mathbf{h}_f^k, \boldsymbol{\omega}^k)$ and $\mathbf{f}_T(\mathbf{h}_f^k, \boldsymbol{\omega}^k)$ are the discretized flow and transport equations calculated using $\mathbf{h}_f^k$ and $\boldsymbol{\omega}^k$, $\Delta \mathbf{h}_f^k$ and $\Delta \boldsymbol{\omega}^k$ are the increments of state variables. The matrix of the system is the Jacobian matrix, which contains the derivatives of flow and transport equations with respect to the state variables.

Picard and Newton-Raphson methods have different properties. Picard's method is a first order method while the Newton-Raphson's method is a second order method. Because of the computation of the Jacobian matrix, the Newton's method is more computationally demanding than Picard's method but these computations can be reused for inverse problem as will be shown in next section. Moreover, the Newton-Raphson's method is more robust (i.e. the method is more likely to converge under unfavourable situations), which is one of the algorithm requirements when doing parameter estimation as stated before. However, the Newton-Raphson's method presents a strong dependence on the initialisation.

Inverse problem

In the inverse problem model parameters are searched as the ones that minimize a certain objective function, J, which depends on the parameters, p, and the state variables.

$$J = J(\mathbf{p}, \mathbf{h}_f, \boldsymbol{\omega}) \tag{8}$$

The minimization of this objective function is performed by Marquardt's method, which implies the computation of the derivatives of h and $\boldsymbol{\omega}$ and J with respect to parameters. The derivatives of the state variables with respect to the parameters are the so called sensitivities.

Computation of sensitivities (variations of state variable with respect to parameters) is an expensive task in the inverse problem. This can be done by parameter perturbation and finite differences between the obtained simulation solutions, by direct derivation or by the adjoint state method. If direct derivation is used, the resulting equation is

$$\begin{pmatrix} \frac{\partial \mathbf{f}_f}{\partial \mathbf{h}_f} & \frac{\partial \mathbf{f}_f}{\partial \boldsymbol{\omega}} \\ \frac{\partial \mathbf{f}_T}{\partial \mathbf{h}_f} & \frac{\partial \mathbf{f}_T}{\partial \boldsymbol{\omega}} \end{pmatrix} \begin{pmatrix} \frac{\partial \mathbf{h}_f}{\partial \mathbf{p}} \\ \frac{\partial \boldsymbol{\omega}}{\partial \mathbf{p}} \end{pmatrix} = \begin{pmatrix} \frac{\partial \mathbf{f}_f}{\partial \mathbf{p}} \\ \frac{\partial \mathbf{f}_t}{\partial \mathbf{p}} \end{pmatrix} \tag{9}$$

It can be seen that the matrix system is the same as in (7). This makes the Newton algorithm suitable when doing parameter estimation since there is no need to compute the system matrix again. An extensive formulation of inverse problem in density-dependent flow and transport can be found in Slooten *et al.* (2002).

Code description

The implementation of the former algorithms is done as an extension of TRANSIN IV code (Medina *et al.*, 2004). TRANSIN IV is a Fortran code for flow and transport modelling under steady and transient conditions. It allows the estimation of any flow and transport parameter.

Discretization

Spatial discretization of the governing equations is done by the finite element method. The finite element mesh can be either one, two or three-dimensional. One-dimensional, triangular, quadrilateral, tetrahedral and triangular prismatic elements are available. Time discretization is made by weighted finite differences.

Linearization

The Newton-Raphson's method and Picard iterations are implemented. There is also the possibility of changing between them within the same time step. This is done according to an iteration number criterion. This is a trial to avoid convergence problems by changing between methods when one of them does not converge.

Solvers

Due to the iterative nature of the algorithm, a set of direct and iterative solvers are included. Direct method is LU decomposition of a band stored matrix. The iterative solver implements the generalized minimal residuals (GMRES) and conjugated gradient stabilized (CGSTAB) methods applied to a sparse matrix included in the WATSOLV package (VanderKwaak *et al.*, 1995). It is also possible to do a preconditioning of the equation system by an incomplete lower/upper factorisation.

Preliminary results

The Henry problem (Henry, 1964) is a known benchmark for seawater intrusion codes. It is based on a case of salt encroachment in a coastal aquifer and tries to reproduce qualitatively the effects of the saltwater intrusion in the aquifer. The problem considers a vertical 2m x 1m section of a coastal aquifer as shown in Figure 2. The upper and lower boundaries are impervious. There is an input flow of 0.066 L/s homogeneously distributed along the left boundary. The equivalent freshwater head is prescribed along the right boundary, following the hydrostatic pressure. Permeability is considered homogeneous and equal to 1.020408E-9 m^2 (equivalent to a hydraulic conductivity of 1.0E-2 m/s). Porosity is equal to 0.35. The problem is considered purely diffusive with a diffusion coefficient of 18.857E-6 m^2/s. The problem was

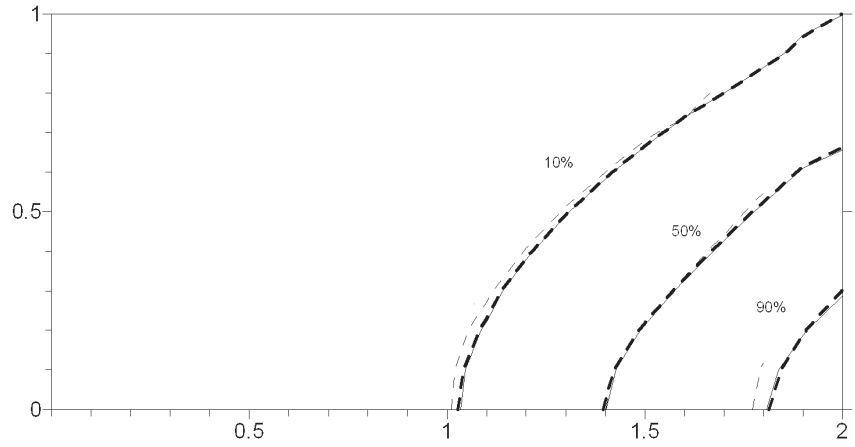

Figure 2. Comparison between TRANSDENS (solid line, identical for both Newton-Raphson and Picard methods), SUTRA (thick dashed line) and the semi-analytical solution given by Segol (1994) (thin dashed line). Isolines corresponding to 90%, 50% and 10% of mixing between freshwater and seawater are shown.

solved over a finite element mesh of 200 regular quadrilaterals with a total of 231 nodes. The method was solved using both Picard and Newton methods.

The results for the stationary situation were compared to the ones of SUTRA code (Voss, 1984) for the isolines corresponding to 10%, 50% and 90% of mixing between saltwater and freshwater (Figure 2). The semianalytical solution of Segol (1994) has also been included. The results obtained with TRANSDENS by the Picard and Newton methods are identical, and their match with the solution given by SUTRA is good. Some small differences in the zones of high salinity can be seen. There the computation of velocities is very sensitive to the buoyancy term. It could also be due to the numerical treatment of the boundary conditions. Also, the position of the wedge toe (defined as the place where the 50% isoline intersect the bottom of the aquifer) is slightly different.

There is also a very good correspondence between TRANSDENS and the semianalytical solution. The deviation of the numerical solutions of both SUTRA and TRANSDENS respect to the semianalytical one are similar.

Conclusions

A code called TRANSDENS for seawater intrusion modelling and parameter estimation has been presented. It is based on a Newton-Raphson algorithm, whose robustness is suitable for calibration and simulation. This algorithm is also appropriate for calibration, since the system matrix can be reused sparing significant computational cost. The Newton-Raphson´s algorithm is also likely to prevent convergence problems. A mixing with Picard method is suggested to help avoiding divergence in some cases.

The verification of the code with the Henry problem gave a good agreement with SUTRA code results for the same problem and with the semianalytical solution.

Inversion of parameters as well as a thorough test of Newton's method will be the issue of future research.

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