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Validation of a finite element code to simulate the coupled problem of salt transport in groundwater

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Abstract

Groundwater contaminations by salt water are frequently observed especially in coastal zones. Moreover, upconing phenomena induced by important pumping is one of the major factor stressing and aggravating the process. After a short synthesis of the coupled equations describing the transport and density dependent flow, a finite element program able to simulate accurately this kind of problems is proposed: the SUFT program (Saturated Unsaturated Flow and Transport model). In order to avoid numerical instabilities, two methods have been introduced in this code covering by this way all the practical cases: the convection dominated as well as the dispersion/diffusion dominated transport cases. The validation procedure for this program has been completed on different well known academic cases for which analytical or numerical results have been previously published by many authors.

1 Introduction

When the introduction of a contaminant into an aquifer causes changes in the density of the water, the groundwater flow is affected. A classical situation is the seawater intrusion in coastal aquifers but also the transport of leachates or salts from industrial waste disposal sites or decantation basins. Major groundwater quality degradations are well known in many coastal aquifers as the contamination by salt water is stressed by upconing phenomena induced by important pumping wells. Previously, many authors have adopted very simple conceptual models neglecting any mixing zone, and assuming that a sharp interface exists between saltwater and freshwater. As mentioned by Galeati et al. [1], many numerical solutions to this sharp interface problem have been proposed in two dimensions between 1977 and 1990 ([2],[3],[4],[5],...), but when dispersion and the vertical flow component become important, a mixing zone is to be taken into account in two or three dimensions. Locally or on a regional scale, the extent of the saltwater intrusion and the salt concentrations in the mixing zone depends on (1) the aquifer geometry, structure, and properties, including hydraulic conductivity, effective and total porosity, dispersivities, effective diffusion coefficient, ...; (2) the solicitations applied to the aquifer including location of the wells, pumping/recharge rates and depths.

In this mixing zone, the flow and the solute transport may be density dependent and the concerned equations are, to some extent, be solved in coupled or partially coupled numerical models. This coupling become more and more necessary as salt concentrations in the water are increasing. Especially, if we are dealing with cases of concentrated brine transport near rock salt formations or induced by accidental leaks of salted chemical leachates from industrial waste sites or decantation basins.

In the cases involving high salt concentrations, Hassanizadeh & Leijnse [6] have indicated that the conceptual model and the assumptions have to be chosen with more careful examination concerning (1) the basic equations, (2) the boundary conditions and (3) the numerical techniques.

After a short synthesis of the equations and of the different possible assumptions that can be taken for modelling purposes, a brief description of the different numerical techniques available to solve the coupled density dependent flow transport problem is proposed. The SUFT code has been tested for validation on different cases described in the literature. As an example, the well-known problem of Henry [7] is solved and the results are compared to those found by other authors and with other finite difference or finite element codes.

2. Equations and conceptualisation

A first assumption consists in considering only porous media where the 'immobile' water effect can be neglected. Consequently, the linear Fickian term describing the transfer coefficient between 'mobile' and 'immobile' water as used by Biver & Dassargues [8] is neglected in the mass balance equation of the ('mobile') water and the mass balance equation of 'immobile' water is not considered. The mass balance equations for water and for salt concentration remain in the system, added to Darcy's law and constitutive equations relating fluid density and eventually fluid viscosity to concentration (isothermal conditions and incompressibility of the fluid are implicitly taken).

Using the classical assumptions concerning the solid fluid interactions, negligible internal friction in the fluid and negligible inertial effects, as developed in Bear & Bachmat [9], the averaged momentum balance equation reduces to the linear Darcy's law:

$$\underline{v} = \frac{\underline{\underline{k}}}{n.\mu}(\underline{grad}\,p + \rho.g\,\underline{grad}\,z) \qquad (1)$$

where all the coefficients or parameters are considered at a macroscopic scale with the Representative Elementary Volume (REV) theory, associated to the continuum approach and the porous medium concept. Here, $\underline{v}$ is the vector of the averaged effective velocity, n the effective porosity or 'mobile' water porosity, $\underline{\underline{k}}$ the tensor of the intrinsic permeability, μ the fluid viscosity, ρ the fluid density, g the acceleration due to gravity and p the fluid pressure. Assuming all the classical hypothesis enumerated by Kipp [10], the mass balance equation for water is generally expressed as:

$$\frac{\partial(n.\rho)}{\partial t} = -div(n.\rho.\underline{v}) + \rho^*.q \qquad (2)$$

where q is the fluid-source flow rate and ρ^* the density of the fluid in the sink/source term [10]: if $q > 0$ then $\rho^* = \rho^*$ (prescribed by the external fluid source) and if $q < 0$ then $\rho^* = \rho$. The left member of the equation (2) expresses the storage in the porous medium of the salted fluid at the density ρ (depending on the salt concentration). If isothermal conditions and negligible compressibility of the fluid are assumed:

$$\frac{\partial}{\partial t}(n.\rho) = n.\frac{\partial\rho}{\partial C}.\frac{\partial C}{\partial t} + \rho.\frac{\partial n}{\partial t} \qquad (3)$$

where C is the mass fraction or solute concentration expressed in terms of mass of solute per mass of fluid. Then in the case of moderated salted water, the fluid density constitutive equation can be reduced to a linear form:

$$\rho = \rho_0.[1 + \beta_C(C - C_0)] \qquad \text{with} \qquad \beta_C = \frac{1}{\rho_0}.\left(\frac{\partial\rho}{\partial C}\right)_{p,T\,cst} \qquad (4)$$

As recalled by Hassanizadeh & Leijnse [6], the fluid viscosity constitutive equation can be written (at 20°C) as :

$$\mu = \mu_0.(1 + 1.85C - 4.1C^2 + 44.5C^3) \qquad (5)$$

The equation (3) is reduced to :

$$\frac{\partial}{\partial t}(n.\rho.g) = n.\rho_0.g.\frac{\partial C}{\partial t} + S_s.\frac{\partial p}{\partial t} \qquad (6)$$

where S_s is the specific storage coefficient due to the volumetric compressibility of the porous medium $S_s = \rho(C).g.\alpha$ with α the volumetric compressibility coefficient (in Pa^{-1}).

Entering equations (1) and (6) in the equation (2), the mass balance equation for the water can be written in terms of the two main dependent variables p and C :

$$S_s.\frac{\partial p}{\partial t} + n.\rho_0.g.\beta_C.\frac{\partial C}{\partial t} = div\frac{\rho(C).\underline{\underline{k}}.g}{\mu(C)}(\underline{grad}\,p + \rho(C).g\,\underline{grad}\,z) + \rho^*.g.q \qquad (7)$$

The solute mass balance equation or transport equation is expressed in the traditional way ([11],[10],...):

$$\frac{\partial(n.\rho.C)}{\partial t} = -div(n.\rho.C.\underline{v}) + div\left[n.\rho.(\underline{\underline{D}} + D_m\underline{\underline{I}}).\underline{grad}\,C\right] + \rho^*.q.C^* \qquad (8)$$

where the processes of adsorption/desorption and decay are neglected, $\underline{\underline{D}}$ is the mechanical dispersion tensor, D_m the effective molecular diffusion coefficient of the solute in the porous medium, C^* the concentration (mass fraction) of the fluid in the sink/source term (equal to C if $q \le 0$).

The mechanical dispersion tensor is defined usually by longitudinal and lateral dispersivities a_L and a_T . In two dimensions, the three components of the dispersion tensor can be reduced:

$$Pe = \frac{|\underline{v}|.\Delta l}{D} \text{ and } Cr = \frac{|\underline{v}|.\Delta t}{\Delta l}$$

where Δl is the dimension of the cell or the element in the concerned direction, Δt the time step, D is the concerned component of the $\underline{\underline{D}}$ tensor. The Peclet number expresses the ratio between advection and dispersion components of the solute transport, the Courant number expresses the advection component of the transport with regard to the discretized size of the cells (elements).
Similarly, using the LAGAMINE code, Biver [15] has established that in transient conditions, the stability of the FUPG method requires that $Cr < 1$, but for convective dominated processes ($Pe > 10$) it is more convenient to use the HELM method with a Courant number as big as possible. The same guidance conclusions are applied for the SUFT code as similar finite element techniques are used.

5. Comparison of results, validation

Results from the SUFT program are compared with solutions published by other authors ([1],[13]) and with results obtained using the HST code. As an example we consider here the well-known Henry's problem, dealing with a uniform isotropic aquifer bounded above and below by impermeable boundaries, receiving a uniform freshwater flow on the left boundary and in contact with sea-water on the right. The data and parameters are chosen as following: hydraulic conductivity $K = 1.10^{-2}$ m/s, effective porosity $n = 0.35$, freshwater flux on the left boundary $q_0 = 6.6\ 10^{-5}$ m/s, density variation $\rho_0.\beta_c \cong 0.7$ and dimensions of the domain with a length/width ratio of 2. Then, two cases are considered: (1) with a constant dispersion with $(D+D_m) = 6.6\ 10^{-5}$ m²/s, and (2) with a variable dispersion $D_m = 0$ and $a_L = a_T = 0.035$m ([1]). Figures 1 and 2 compare our results with those obtained by other authors and with the HST.
One of the features influencing the computed solutions near the right boundary is clearly the way of treating the sea-water boundary. Usually, a prescribed concentration is chosen when the flow is directed inward and a zero dispersive flux when the flow is directed outward. Galeati et al. [1] and the HST program [10] can treat this problem assigning the appropriate boundary conditions according to the computed direction of the flow. Using the LAGAMINE code, Munhoven [13] has assumed that the flow is entering only by the lower quarter of the boundary. Following the same kind of reasoning, and as it was also suggested by Yeh [17], we have considered that only the upper third of this boundary is crossed by outward flows so that we can prescribe the concentration on the rest of the boundary without making a big error. However, the results show that differences are observed near this boundary. Elsewhere in the domain, the computed isoconcentration lines are very similar to those found by other authors and using the HST.
In the LAGAMINE code, the Boussinesq approximation was assumed and moreover only a partial coupling was made, updating the coefficients at the end of chosen time steps. In order to be able to treat problems involving brines and more salted waters, a complete coupling has been considered in the SUFT program on basis of the method exposed by Yeh [17].
The SUFT output files are tailored to be treated immediately by the IBM Visualisation Data Explorer (DX).

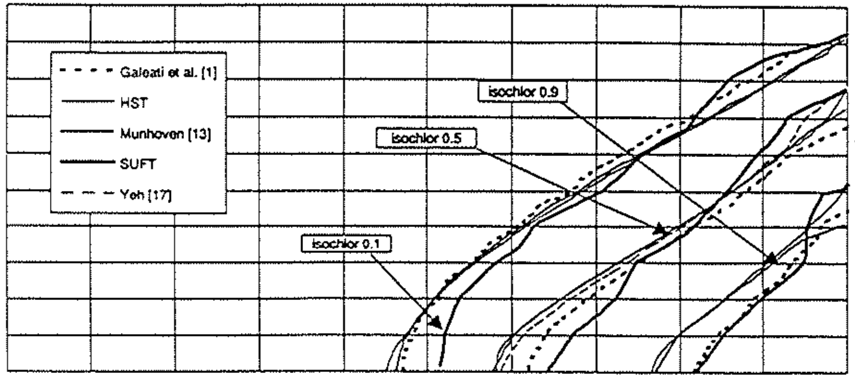

Figure 1 : Computed results for the Henry's problem with a constant dispersion.

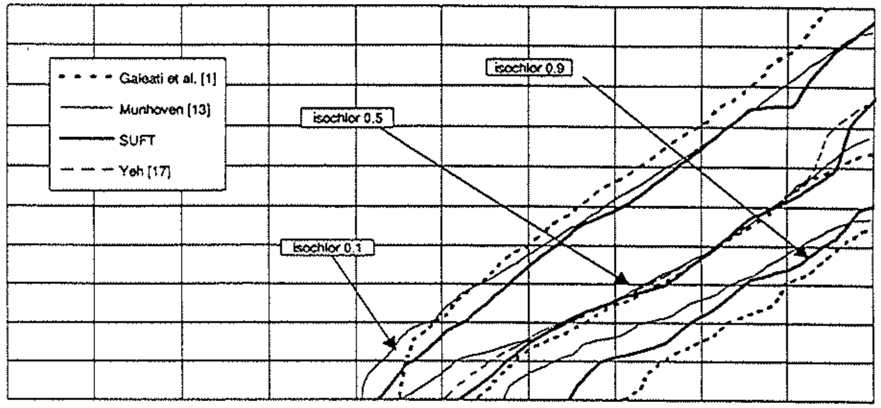

Figure 2 : Computed results for the Henry's problem with a velocity dependent dispersion.

6. Conclusions and future prospects

Developing our new research code, many idea and lessons were drawn from the experience of development of the LAGAMINE code by Biver [15] and Munhoven [13]. The SUFT code has been validated for flow transport problems coupled by the density effect. In the future, other non linear equations of flow and transport will be implemented in this research and experimental software; we are thinking particularly to multiphase flows and especially to flow and contamination in the partially saturated zone.

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