DEVELOPMENT OF A COUPLED FLOW AND TRANSPORT 3D MODEL FOR SIMULATING SEAWATER INTRUSIONS IN COASTAL AQUIFERS

G. Carabin[1] & A. Dassargues[1 & 2]
[1] L.G.I.H., University of Liège, Belgium
[2] Hydrogeology, K.U.Leuven, Belgium

ABSTRACT

In coastal zones, the well-known seawater intrusions are stressed by freshwater drainage or pumping in the upper parts of the aquifers. A finite element program able to simulate the mixing zone in 3D is proposed : the SUFT3D code (Saturated Unsaturated Flow and Transport 3D model). The coupled equations describing the transport and density dependent flow are implemented assuming the "classical Boussinesq approximation". A mixed formulation (water content - pressure head) is used in the flow equation to solve the mass conservation problems in the unsaturated zone. The simulated transport processes are advection, diffusion, dispersion, linear degradation, adsorption (with linear, Langmuir or Freundlich isotherm) and eventual immobile water effect. Different theoretical tests have been performed to validate the code by comparison to cases described in the literature. Then the complexity of the tests is progressively increased in order to check the ability of the code for modelling real practical cases : confined and unconfined aquifers, small- and large-scale domains, homogeneous and heterogeneous groundwater flow and transport parameters. Simulations including river interactions with groundwater are also successfully performed.

INTRODUCTION

In the framework of the SALMON project (Sea Air Land Modelling Operational Network) supported by the IBM International Foundation, integrated water quantity and quality problems are addressed in coastal zones (Dassargues et al., 1996). This research project consists mainly in introducing natural junctions between three existing models (ocean, river and groundwater) to form one single integrated model, able to describe water and contaminant fluxes in a whole system, at regional scale, including marine, river and groundwater inputs. Concerning groundwater part, the first step of the research was devoted to develop the SUFT3D (Saturated Unsaturated Flow and Transport in 3D) groundwater model and to check its efficiency and accuracy in reproducing typical situations of seawater intrusions. Some of the most significant results of these tests are given hereafter.

EQUATIONS AND THEORETICAL BACKGROUND

In order to be able to study very different actual 3D cases where the heterogeneity and the dispersion cannot be neglected, we have adopted the concept of mixing zone. The fluid-water-density may vary in space and time as a function of changes in concentration, temperature and pressure. This leads to coupled or partially coupled groundwater flow and transport equations with non linear parameters. Generally coupled equations containing cross-coupling terms can be derived from a rigorous thermodynamic approach (Hassanizadeh & Leijnse, 1988). This last approach is only needed for cases of high salt concentration (proximity of salt domes or salt formations). In this study, the classical approach of balance equations expressed for an unitary volume of the porous medium is used and summarised here below.

Another 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 (1993) is neglected in the mass balance equation of the ('mobile') water and the mass balance equation of 'immobile' water is not considered.

In isothermal and saturated conditions and with the classical assumptions concerning the solid-fluid interactions, negligible internal friction in the fluid and negligible inertial effects, as developed in Bear & Bachmat (1990), the averaged momentum balance equation is reduced to the linear Darcy's law for an aquifer:

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

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.

The mass balance equation for water is generally expressed as :

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

where S is the degree of saturation, $\underline{V_S}$ the velocity of the deformable surface, q the internal sink/source flow rate, ρ^* the density of the fluid in the sink/source term. If $q > 0$ then $\rho^* = \rho^*$ (prescribed by the external fluid source) and if $q < 0$ then $\rho^* = \rho$. In the unsaturated zone, the expression (1) of the averaged effective velocity must be divided by the degree of saturation (S). Additionaly the intrinsic permeability depends on S.

The solute mass balance equation or transport equation is expressed by :

$$\frac{\partial(n.\rho.C)}{\partial t} = -div(n.\rho.C.\underline{v}) - div(\theta\rho C\underline{V_s})$$
$$+ div\left[n.\rho.(\underline{\underline{D}} + D_m\underline{\underline{I}}).\underline{gradC}\right] + \rho^*.q.C^* \qquad (3)$$

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

The variations of the fluid density and viscosity with the solute concentration are usually expressed by polynomial or exponential expressions. In the case of moderated salted water, the fluid density constitutive equation can be reduced to a linear form :

$$\rho = \rho_0.[1 + \beta_C(C - C_0)]$$

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

Using relative concentration (Cr) defined by $Cr = (C - C\min)/(C\max - C\min)$ with $C\min = C_0$, the equation (4) is written

$$\frac{\rho}{\rho_0} = 1 + \varepsilon C_r$$

$$\text{with} \quad \varepsilon = \frac{\rho_{\max}}{\rho_0} - 1 \qquad (5)$$

The equations (2) and (3) are mainly coupled through the fact that the variation of density in function of the concentration $\rho(C)$ will influence the groundwater flow effective velocity $\underline{v}$ (equation 1), in a way which renders both equations (2) and (3) non linear.

Many authors (Gartling & Hicokx, 1985; Hassanizadeh & Leijnse, 1988; Galeati et al., 1992; ...) do not consider the system of equations (2) and (3) in its whole complexity. They use an approximation known as the 'Boussinesq approximation' and additionaly they are not interested in the partially saturated zone. The 'Boussinesq approximation' states that the density variation is to be considered only in the Darcy's law equation (1), reducing the water mass balance equation (2) to a volumic balance equation :

$$div\left[\frac{\rho(C)g\underline{\underline{k}}}{\mu(C)}(\underline{grad}(h)+\frac{\rho(C)}{\rho_0}\underline{grad}(z))\right] + \frac{\rho^*}{\rho_0}q = (\rho_0 g\alpha)\frac{\partial h}{\partial t} \tag{6}$$

where α is the volumetric compressibility coefficient of the porous medium. In terms of equivalent piezometric heads of freshwater ($H = h + z = \frac{p}{\rho_0 \cdot g} + z$) we obtain using (5):

$$div\underline{\underline{K'}}\left[\underline{gradH} + \varepsilon\,\underline{gradz}\right] + \frac{\rho^*}{\rho_0}q = (\rho_0 g\alpha)\frac{\partial H}{\partial t} \tag{7}$$

where $\underline{\underline{K'}} = \frac{\rho(C)g\underline{\underline{k}}}{\mu(C)}$ is the 'modified' tensor of the hydraulic conductivity.

The equation (7) shows that when dealing with non ideal solutes, the fluid fluxes are not orthogonal to the equipotential lines. Using this system is generally qualified, in the literature, as adopting the 'generalised Boussinesq approximation'. Moreover, if K' is assumed as constant with regard to the solute concentration, one speaks generally of the 'classical Boussinesq approximation'.

Munhoven (1992) has shown that this last approximation can be accepted when awaited salinity variations are limited to 50 0/00 (more than usual contrast between freshwater and seawater) under pressure variations not exceeding 3.0 10^8 Pa (approximately 3000 atm). Then, if it is assumed additionally that the porous medium is incompressible, the obtained flow equation for a confined aquifer is similar to the Laplace equation :

$$div\underline{\underline{K'}}\left[\underline{gradp} + \rho(C)g\ \underline{gradz}\right] + \rho^* gq = 0 \tag{8}$$

and the coupled transport equation is written :

$$-div(C\underline{v}) + div\left[(\underline{\underline{D}} + D_m\underline{\underline{I}})\underline{gradC}\right] + \rho^* C^* q' = \partial C/\partial t \tag{9}$$

where $q' = q/n\rho_0$ is the modified sink/source term. The equations of this system being coupled, the equation (8) can be considered as a transient equation due to the time variation of the solute concentration.

SUFT3D

The SUFT3D code developed at the LGIH of the University of Liège can treat full 3D real cases in steady or transient conditions for both confined or unconfined aquifer. This is a finite element code solving the groundwater flow (which can be density dependent) and the transport of a dissolved contaminant through the saturated and unsaturated porous media. Linear interpolation functions are used in elements of eight, six or four nodes.

The main flow variable is the pressure head (h). It is well known that this formulation in terms of the pressure head can cause some problems of mass conservation when a part of the unsaturated zone is modelled explicitly in the groundwater model (Milly, 1985). Problems come from the difficulty induced by the adequate estimation of the generalised storage coefficient which is highly non linear in this partially saturated zone when applying the mass balance equation on the discretized domain. To solve the mass conservation problems in the unsaturated zone , the mixed formulation (water content - pressure head) is used in the flow equation as proposed by Celia et al. (1990). The velocities are calculated by applying directly the finite element method to the Darcy's equation (Yeh, 1981). They do not result from the derivatives of the computed pressure field. This method reduces strongly errors in the mass balance. Additionally it seems to be particularly convenient to simulate density dependent groundwater flow when the vertical component of the velocity can be non negligible as in water table aquifers (Strobl & Yeh, 1994). A traditional Galerkin finite element method is used. For the transport equation, an Eulerian Upstream (EUM) or Hybrid Eulerian-Lagrangian (HELM) finite element method can be used in the cases of high Peclet numbers (<10 with EUM and unlimited with HELM) and high Courant numbers (only HELM). However, up to now the HELM is only available in the SUFT3D code with hexahedral finite elements. The well-known WATSOLV solver package (Van der Kwaak et al., 1997) is used to insure efficiency and reliability. The solving method implemented in WATSOLV is an iterative process which is preconditioned using an Incomplete Lower-Upper factorisation. The particularity is that the iterative process is accelerated using one of two algorithms : GMRES (Generalised Minimal RESidual) or Bi-CGSTAB (Biconjugate Gradient STABilised) (Saad, 1996).

TESTS

The SUFT3D code has been tested on different cases described in the literature. The tests on the problem of Henry (1964) have been published previously by Dassargues (1994). Then, various tests approaching more realistically actual conditions have been made with the SUFT3D, introducing step by step more complex situations.

Seawater intrusion in a water-table aquifer

A test problem for seawater intrusion in an unconfined aquifer was proposed by Huyakorn et al. (1987). The data, parameters and boundary conditions of the modelled domain are given on figure 1. The seawater boundary is on the left side and due to the density effect a seawater intrusion is observed. A freshwater inflow is considered on the right boundary in the same time that an important recharge occurs on the top of the aquifer.
Computed results from SUFT3D are compared with those from Huyakorn et al. (1987), Galeati et al. (1992) and Strobl et al. (1994) (figure 2). A good agreement is found for the computed isochlor $Cr = 0.5$ (relative concentration) except comparing with the solution proposed by Huyakorn et al. (1987). It has been demonstrated by Strobl et al. (1994) that a too rough approach was chosen by these authors for calculating nodal velocities with the needed accuracy. Other small differences between the different computed results can generally be explained by the use of different solving methods, meshes and interpolation schemes. Comparing with results from Galeati et al. (1992), significant differences are observed in the upper part of the domain. It is due to the fact that the chosen top boundary condition is not similar. They have chosen a (C = 0) Dirichlet boundary condition for transport where, according to our analysis, this condition is in fact not appropriate to represent an actual situation where an unconfined blackish aquifer is recharged by freshwater. The recharge brings freshwater which mixes with ground-water. This does not mean automatically that the relative salt concentration in the aquifer is zero near the top boundary. The boundary condition proposed by Huyakorn et al. (1987) (figure 1) is more appropriate : the mass fluxes are equal to advective fluxes when the flow comes into the domain with the concentration C*. It is closer to the reality, and hence-forward, it will be adopted in all simulations to define the boundary conditions on the top of the unconfined aquifer.

Seawater intrusion in an homogeneous large-scale water-table aquifer

The dimensions of the modelled domain and the boundary conditions are presented on figure 3. The parameter values are identical to those of the previous case. No freshwater input is imposed on the left boundary because the aquifer is supposed in piezometric equilibrium with the outside conditions.
The previous results have shown a diffusive-dispersive front of salt water which is not longer than 100 meters. Since similar hydrogeologic parameters are used in this case, it is necessary to use elements not larger than 50 m in order to represent accurately the salt water front. If larger elements are chosen, numerical dispersion will appear inducing enlarged salt water front compared to the actual front.
The computed intrusion of salt water for this case is presented on figure 4a. The simulated dispersive front is very similar to the results found in the previous case. A comparison can be made because the computed inflow of fresh water at a distance of 200 meters from the coastal boundary is nearly equivalent to the fresh water inflow prescribed in the previous

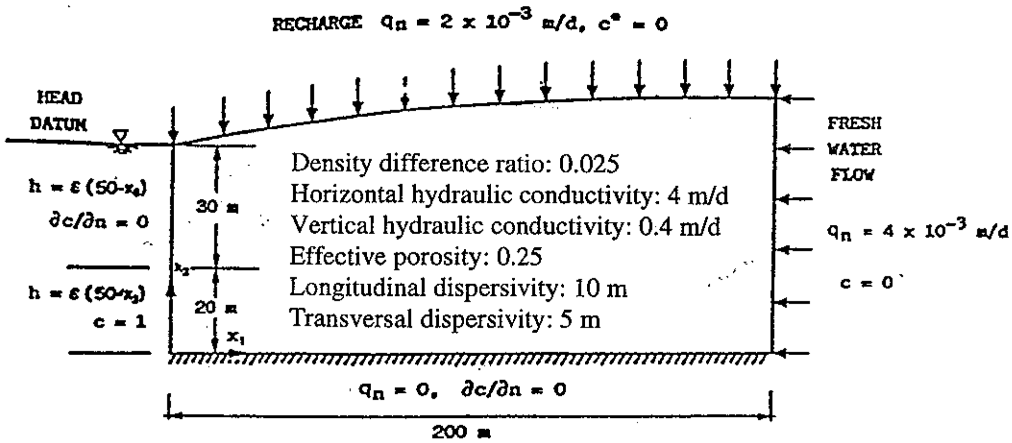

Figure 1 : Definition of the seawater intrusion problem studied by Huyakorn et al. (1987).

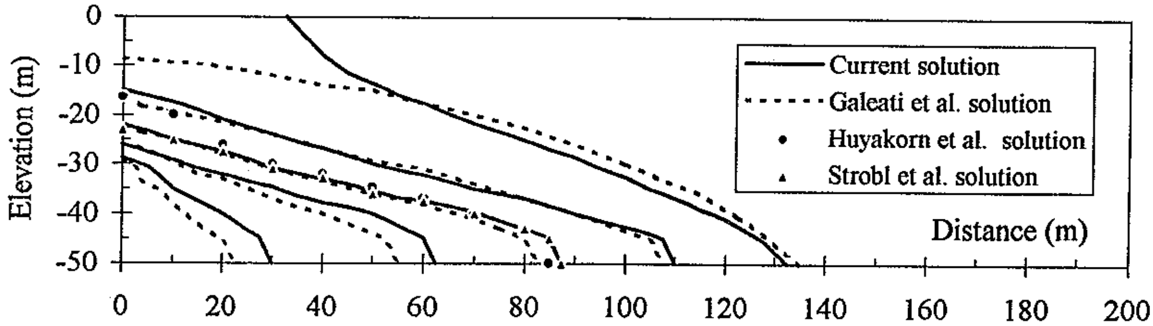

Figure 2 : Comparison of results (isochlor lines 0.1; 0.3; 0.5; 0.7; 0.9).

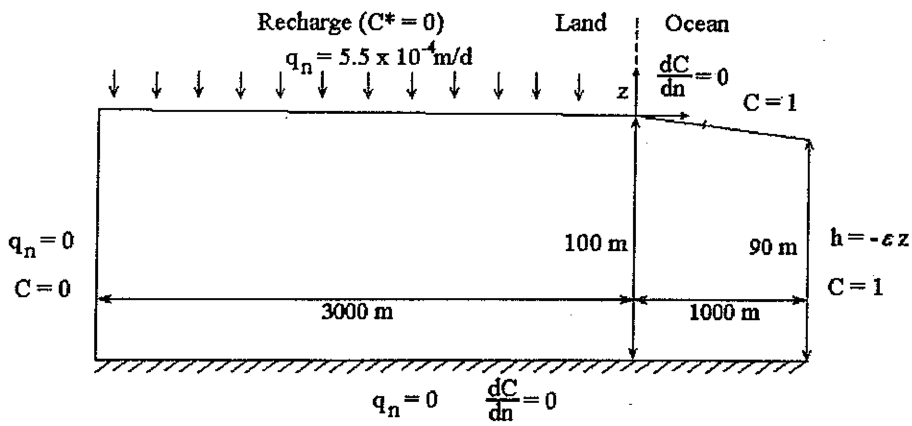

Figure 3 : Definition of the seawater intrusion problem for a large scale aquifer.

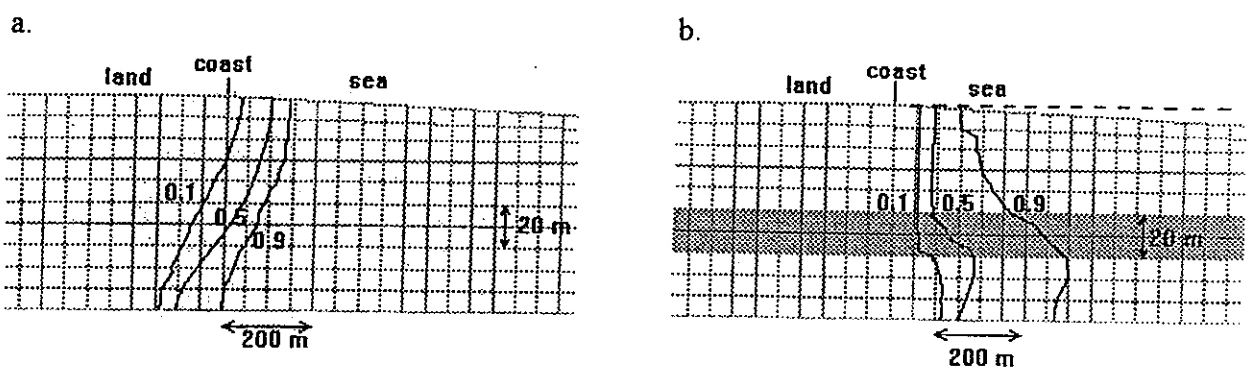

Figure 4 : Zoom on the results for the homogeneous case (a), and for the heterogeneous case (b)

case. However, the seawater intrusion is more important because of the 100 meters thickness of the domain in place of the 50 meters. Another difference comes from the fact that the piezometric head and the unit relative concentration are no more prescribed under the coastline but on the continental shelf and thus the pressure head decreases faster upwards under the coastline. This fact explains that the dispersive front appears rather down at this place. It can be pointed out also that Dirichlet conditions ($C = C^*$) cannot be prescribed on the whole continental shelf. In order to allow freshwater outflow, Neumann condition for transport ($dC/dn=0$) must be prescribed on a part of the shelf.

Seawater intrusion in an heterogeneous large-scale water-table aquifer

The same domain is modelled but distinguishing a less pervious horizontal layer separating two aquifer layers. Thus unconfined (upper aquifer) and confined (lower aquifer) conditions are studied simultaneously in the same domain. The parameters of the more permeable layers are the same as those used previously. The horizontal and vertical hydraulic conductivity values of the less permeable layer are taken with a ratio of 0.015 with regard to the values in the two aquifers and a 0.15 effective porosity value has been taken (instead of 0.25 in the aquifer).
On figure 4b, the results show that in the lower aquifer, the freshwater goes farther under the ocean. It is due to the fact that the piezometric heads do not decrease as sharply as in the unconfined aquifer. However, the saltwater intrusion in the unconfined aquifer is still influenced by input coming from the lower aquifer.

Seawater intrusion in an aquifer which is drained by a river

The efficiency of the river boundary condition implemented in the SUFT3D was also checked. Results of these tests can be found in the technical report of the SALMON project (Nihoul et al., 1996). Hereafter, only the theoretical case of a seawater intrusion in an aquifer drained by a river will be described.

The chosen domain is 3 km long (2 km in land and 1 km under ocean), 2 km wide and 0.1 km thick. A 300 m wide river is located in the middle of the considered domain. A finite element meshing network has been built with 100 x 100 x 10 m basic elements, for a total of 8320 elements and 9735 nodes. The mesh, parameters, and boundary conditions are given on figure 5 where the elements in contact with the ocean are in dark grey and those in contact with the river in white.
The lateral boundaries of the domain are taken impervious because the effects of the draining river on the aquifer are supposed negligible at that distance and consequently the groundwater flow can be considered as mainly parallel to those boundaries. The other boundary conditions are similar to these prescribed in the case of figure 3. No flux is imposed on the upward (left) boundary (which is located 2 km inland) because the aquifer is supposed in piezometric equilibrium with the river (which has a low gradient). In these conditions the only water fluxes from the aquifer to the draining river can be considered as orthogonal to the river and thus parallel to the upward boundary.
The results of the flow and transport computations with the SUFT3D code are shown on figures 6. The river drains the aquifer and consequently the isopiezometric surfaces (in equivalent freshwater piezometric heads) are approximately vertical and parallel to the river direction in the areas where the ocean is too far for having an influence on the groundwater flow. Approaching the ocean boundary, the isopiezometric surfaces become progressively horizontal and parallel to the coastline due to the density effect of the saltwater. Near the river, the local decrease of the piezometric heads induced by the drainage of the river is aggravating the salt water intrusion under the river and at the river mouth. Considering vertical cross sections, the computed isochlor $Cr = 0.5$ is found 500 m inland under the river and only 100 m inland when the cross section is located farther from the river. The salt water intrusion under the river is limited thanks to the lateral fresh groundwater flow going towards the draining river.

Fresh water recharge at the top: 0.00055 m/d
Bottom river transfer coefficient (K_r / e_r): 0.1 d^{-1}
Gradient of the river: 0.01 %
Density difference ratio: 0.025
Horizontal hydraulic conductivity: 2 m/d
Vertical hydraulic conductivity: 0.2 m/d
Effective porosity: 0.15
Longitudinal dispersivity: 20 m
Transversal dispersivity: 10 m

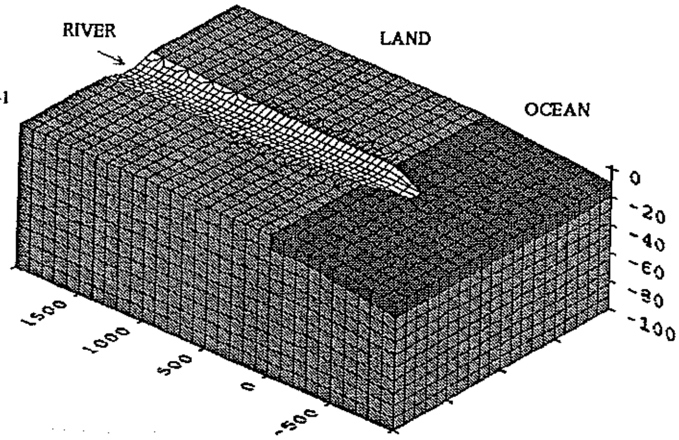

Figure 5 : Definition of the parameters and modelled domain for computing simultaneous groundwater-river and groundwater-seawater interactions

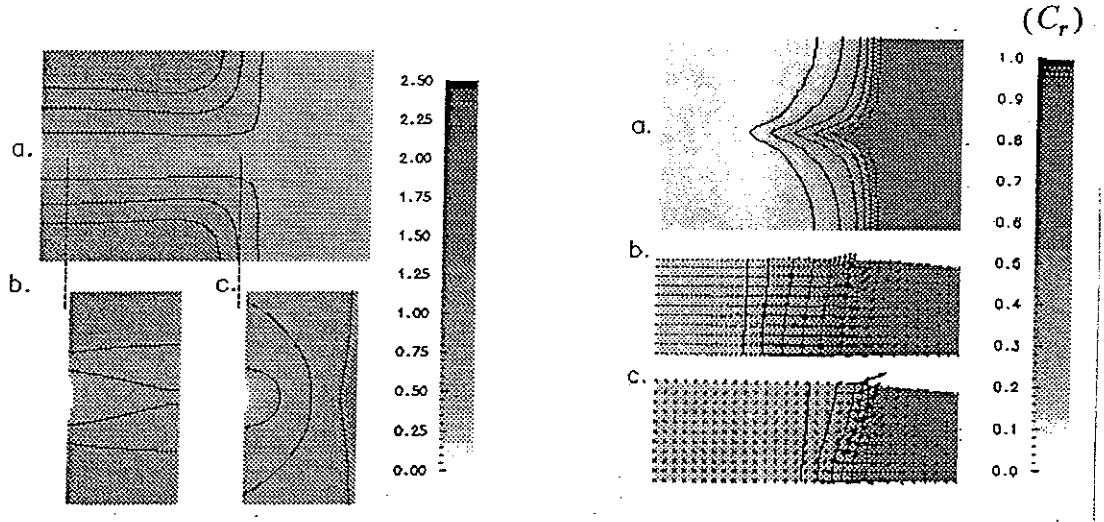

Figure 6: SUFT3D results for a seawater intrusion in an homogeneous aquifer drained by a river.
- Results for groundwater flow (on the left) : horizontal cross-section at -50 m (a) and vertical cross-sections (b and c) with the isopiezometric surfaces in equivalent freshwater piezometric heads 0.5, 1.0 and 1.5 m.
- Results for transport (on the right) : isoconcentration lines 0.01, 0.1, 0.3, 0.5, 0.7 and 0.9

CONCLUSIONS

Tests have been carried out in different situations with increasing complexity to approach practical situations of seawater intrusions : confined and unconfined aquifers, local and regional domains, homogeneous and heterogeneous aquifers, influence of the river interaction. All the results of the modelled seawater intrusion problems cannot be compared to analytical or numerical results of the literature but, when they can, they prove the efficiency and the reliability of the SUFT3D code. The tests have provided results which seems logical with the physic of the new studied problems. The results of the innovative tests with groundwater exchanges with both the river and the ocean are particularly interesting to understand the flow-transport dynamic in groundwater systems of the coastal zones especially when groundwater-river interactions are taken into account.

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