Salt Water Intrusion into Freshwater Aquifers : A 3D Modelling and a Parallel Algorithm

J.M. Crolet and F. Jacob

Laboratoire de Calcul Scientifique
Université de Franche-Comté
25 030 Besançon , France

Abstract. This paper deals with the numerical modelling of salt water intrusion into freshwater aquifers. Difficulties of the problem are presented, analysed and a possible remediation is described. The case of situation induced by systems of very large size is also investigated and a new parallel algorithm is provided.

1. INTRODUCTION

Many population living in coastal areas are dependant on freshwater resources. However, this resource is subject to a minor or severe seawater intrusion. Countries facing with such a problem include France, Belgium, the Netherlands, Greece, United Kingdom, Marrocco and Australia.

The study of seawater intrusion is not new. The first model was introduced in 1888 by Ghyben from the Netherlands, followed by Herzberg in 1901 from Germany and since has been known as the Ghyben-Herzberg model. This model was very simple and it didn't take into account convection, dispersion and diffusion phenomena responsible for salt water intrusion.

Since the develpoment of Ghyben-Herzberg model, numerous solutions for this problem have been proposed by various investigators. However, an important part of these solutions are based on a two dimensional representation and they don't take into account phenomena which can be considered as three dimensional.

2. MODELLING

Our model has been developped in 1993 (Jacob *et al.*, 1995), in order to simulate flow and solute transport in saturated porous media with density dependent groundwater flow and solute transport. In this paper, we present a study of numerical problem that we have encountered in such three dimensional modellings. The fluid mass balance equation in saturated porous media, taking into account two primary dependant variables, the pressure P(x, y, z; t) and the concentration C(x, y, z; t), can be expressed as :

$$S \frac{\partial \rho}{\partial t} + (\varepsilon \frac{\partial \rho}{\partial C}) \frac{\partial C}{\partial t} - \nabla [\frac{\varepsilon \rho k}{\mu} (\nabla P - \rho g)] = 0$$

where x, y, z are coordinate variables (L), t is the time (T), S is the specific pressure storabivity (LT^2M^{-1}), ε is porosity (dimensionless), ρ is fluid density (ML^{-3}), μ viscosity ($ML^{-1}T^{-1}$), k is solid matrix permeability (M^2) and g is gravitational acceleration (LT^{-1}). This equation is written without second member because the fluid mass sources are considered as boundary conditions.

The solute mass balance equation for a single species stored in solution is expressed as :

$$\frac{\partial (\rho \varepsilon C)}{\partial t} + \nabla [\varepsilon \rho q C] - \nabla . [\varepsilon \rho (D_M I + D) . \nabla C] = 0$$

where D_M (L^2T^{-1}) is apparent molecular diffusivity of solutes in solution in a porous medium, I is the identity tensor (dimensionless), D (L^2T^{-1}) is the dispersion tensor and q is the average velocity (LT^{-1}) based on the Darcy's law.

It can be noted that, contrary to usual equations published in literature, there is no second member in the equations. In fact, the fluid mass sources are considered as boundary conditions on the mesh. A variational formulation of the above equations has been developped with relevant initial and boundary conditions.
The convection-diffusion equation is an example of hyperbolic type equation. Common methods for

numerical solution of such an equation are the method of characteristics (which is not easy to extend in 3D case), the finite difference method (easy to program but may present some difficulties if the solution is not smooth), the finite volume and the finite element methods. The finite volume method is equivalent (in precision) to a finite element method of degree 1; it preserves the positivity of the solution but it doesn't allow a finest computation of the flux through the faces of the elements.

The software EOS is based on the solution of the above two non linear partial differential equations, which are dependant on each other by the concentration C and the density ρ. A FEM (Finite Element Method) is used with a 20 nodes hexaedron. An interpolation of degre 2 allows us a better computation of the fluid velocity. The symmetric linear system obtained with the flow equation is solved by a conjugate gradient method preconditionned by a SOR method with optimal parameter. The nonlinear system generated from the mass balance equation is solved by the double conjugate gradient method where the matrix is preconditionned by a LU decomposition. The time dependance is solved by an implicit Euler scheme.

3. DESCRIPTION OF THE HENRY'S TEST

For a validation of the software EOS, we have used the bench'mark of the Henry's problem which is an academic case of salt water intrusion into freshwater. The following domain is considered (figure 1).

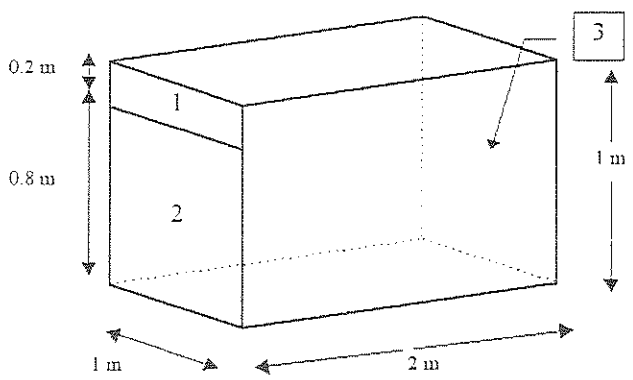


Figure 1 : Geometrical domain for Henry's problem

The boundary conditions and the physical parameters are summarized in Tables 1 and 2 respectively.

TABLE 1 : Boundaries conditions

on face 1	$\vec{\nabla} C . n = 0$ piezometric level = 1 m
on face 2	C = 0,0357 piezometric level = 1 m
on face 3	C = 0 inflow rate = $6.66.10^{-2}$ $kg.s^{-1}$

TABLE 2 : Physical parameters

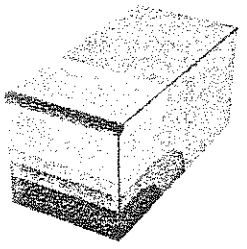
$\varepsilon = 0.35$	$k = 1.020408\ 10^{-9}\ m^2$
$\mu = .001\ kg.\ m^{-1}.s^{-1}$	$\partial\mu/\partial C = 0.0$
$\rho_S = 1025 kg.m^{-3}$	$\rho_0 = 1000\ kg.m^{-3}$
$\partial\rho/\partial C = 700\ kg.m^{-3}$	$D_M = 6066.10^{-6}\ m^2.s^{-1}$
$S = 10^{-7} m.s^2\ kg^{-1}$	D =0.Id

The goal of this work is not the solution itself which is in accordance with the Henry's solution but the quality of this solution. In a numerical modelling based on an usal or Galerkin finite elements method, some negative values will be generated, in the Henry's test, for too many nodes. The major interest of this test case lies in the nature of the flow: indeed, the freshwater that is coming from the upstream face (n° 3) and discharging through the downstream face (n° 1 and 2) is disturbed by salt water intrusion located in the lower part of the downstream face. This intrusion operates naturally by the density contrast. However it is important to note that this numerical phenomenon has not been observed in more realistic cases and specially in cases where the flow is smooth (uniform in its direction and its velocity).

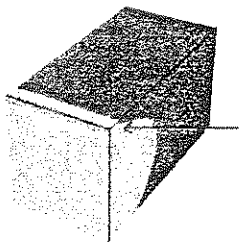
Among these possible remediations, a solution consists in a SUPG (Streamline Upwind Petrov Galerkin) optimized method, it is to say a SUPG method where the parameter of the upwind scheme is optimized. This method, more precisely described by Johnson (1994) can be easily implemented. It only necessitates a modification of the basic functions. If one notes φ the basic functions used in the Galerkin's method, the type of basic functions used in the SUPG method is

$\varphi+\alpha q.\nabla\varphi$ where q is the flow velocity, $\nabla\varphi$ the gradient of φ and α a parameter to be determined (Brooks *et al.*, 1982). Note that if this parameter is zero, the SUPG method becomes the classic finite element method (Galerkin's method). Such a method allows to take into account, for each element, the upstream flow. Then it is useful to research the optimal value for this parameter α and therefore to define a criterion for optimization. It has been demonstrated that the minima of negative values could be an efficient criterion (Crolet et *al.*, 1995)..

It is clear that the optimization of the use of an upwind scheme improves results, but it is not sufficient because some negative values are always obtained during a few time steps. It can be observed that these negative values are always localized forwards of the front line, in the upper part of the domain. The interest of this Henry's test case lies in the fact that the streamlines are not unidirectionnal and that there exists a "shear" in the flow: normally, the freshwater is moving from the upstream face (3) to the downstream face (2). The salt water moves into the domain from downstream to upstream. Therefore, there is in the vicinity of the front line a zone in which there is inversion of the flow direction (figure 2).



2.1 x-component



2.2 z-component

Figure 2 : Representation of the flux by its components

Figure 2 represents the flux inside the domain. This stream has 3 components (one for each axis) and only the components along the x and z axis are interesting. The field of the x-component is regular, very smooth, on the contrary, the field of the z-component present an important gradient especially in the top and in front of the domain (see the arrow).

The Henry's problem which is defined with the initial conditions described in this paper, is very academic. In fact, it contains a strong discontinuity: a situation, where there is for the concentration of solute at the initial time, a zero value inside the domain and a strictly positive value on a face has no physical reality. In a mathematical point of view, an assumption of continuity in the boundary condition is not verified. This is the reason why there is a numerical perturbation (perfectly controlled) in the solution for the solute concentration during a few time steps. In more conventional or more realistic problems, there is no such disturbance.

4. DOMAIN DECOMPOSITION AND PARALLEL COMPUTING

Parallel computing can be introduced at two levels. The software itself can be parallelized and can work on several processors. This parallelization is not the goal of this presentation. Here, a computer is a machine (sequential or parallel) were the software is running. Now we describe the use of several computers running together with the same software and linked for communication in order to solve a problem discretized to a very large system.

The problem is defined on a domain Ω which is divided into many other sub-domains (for instance 100 sub-domains) Ω_i without overlapping. The PDE defined on Ω can also be defined on each subdomain Ω_i . The difficulty is to take into account the boundary conditions (essentially the Dirichlet condition). In fact, these conditions are only defined for the global problem and cannot be reported on each Ω_i . So the problem which is written on each Ω_i is not mathematically well defined because the unicity is not guaranted. In order to simplify the presentation we consider only the flow problem with the unknown P. The equation (1) is similar to Laplace equation and the solution is of the form P+a where the value of the constant a is determined from the Dirichlet condition.

The equation (1) can be written on the sub-domain Ω_i and computed to obtain a solution Π_i . If we note P_i the restriction of the solution P of the global problem to the sub-domain Ω_i , we have : $P_i = \Pi_i + a_i$ where a_i is a constant defined on the sub-domain Ω_i .

On the interface between two sub-domains Ω_i and Ω_j , we obtain two possible solutions: Π_i and Π_j .So, the computation of local solutions introduces a jump $w_{ij} = \Pi_i - \Pi_j$ on the interface $\delta\Omega_i \cap \delta\Omega_j$.

Now, let us imagine we have solved equation (1) on all the sub-domains, we have computed jumps on all possible interfaces and the global solution will be obtained when the values of coefficients a_i will be determined. But these coefficients are solution of a global optimisation problem which generally has a "small" size.

5. CONCLUSIONS

The physical problem of aquifer contamination (or remediation) is the center of major questions in environmental studies. Numerical simulation needs a robust scheme and the solution on a large size domain. A scheme will be more robust if it respects the physical aspect of the problem; such a possibility is given by the SUPG method. Actually, parallel computing is, without any doubt, the only one possibility to solve very large scale problem in an acceptable computing time. The software can be parallelized, but it is important to parallelize the problem. The method of domain decomposition is a possible investigation but it needs to adapt the usually used algorithms. The major advantage of such a method is the possibility to have different meshes in different sub-domains and to pursue computation on a sub-domain only if there is a change in its boundary conditions.

6. REFERENCES

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