Modeling strongly coupled groundwater flow and solute transport in porous medium: re-evaluation of the salt dome flow problem

A. Younes, Ph. Ackerer and R. Mose

Institut de Mécanique des Fluides, Université Louis Pasteur - CNRS - UMR 7507, 2, rue Boussingault, 67000 Strasbourg, France

E-mail: name@imf.u-strasbg.fr

Abstract

Case 5, Level 1 of the international HYDROCOIN groundwater flow modelling project, is an example of idealised flow over a salt dome. Several independent teams simulated this problem using different models. Results obtained by different codes can be contradictory. We develop a new numerical model, TVDV-2D based on the mixed hybrid finite elements approximation for flow, which provides a good approximation of the velocity, and the discontinuous finite elements approximation to solve advection equation, which gives a good approximation of concentration even when dispersion tensor is very small. We use the TVDV-2D code to simulate the salt dome flow problem.

In this paper we study the effect of dispersion and we compare linear and non-linear dispersion equations. We show the importance of the discretization of the constant concentration boundary condition on the extent of recirculation and the final salt distribution. We study also the salt dome flow problem with a more realistic dispersion (very small dispersion tensor). Our results are different from prior works with regard to the magnitude of recirculation and the final concentration distribution. In all cases, our results show recirculation in the lower part of the domain. When the dispersion tensor becomes very small, the magnitude of recirculation is small.
1 Introduction

Study of radionuclide transport (for safety reasons) in the geosphere requires an understanding and prediction of groundwater flow and transport near salt domes. Often such predictions need to be made for several thousands of years. It is therefore necessary to use mathematical models. Case 5, Level 1 of the international HYDROCOIN (OECD, 1988) groundwater flow modelling project, is an example of idealised flow over a salt dome. Many numerical models based on finite differences (FD), finite elements (FE), integral FD or method of characteristics were used to simulate this test case.

In the following, we briefly present our strategies to solve numerically this non-linearly coupled equations for the salt dome problem. These strategies are implemented in a 2D simulator TVDV-2D (Transport with Variations of Density and Viscosity) used to solve the salt dome test case. We study the effect of dispersion/molecular diffusion and the influence of boundary conditions discretization. We also study the salt dome problem with very small dispersion tensor (more conforming to coefficients used in groundwater).

2 Governing equations and numerical schemes implemented in TVDV-2D

The transport of solute in a porous medium in case of variable fluid density can be described by the fluid and solute mass balances, generalised Darcy’s law and equations of state for the liquid density and viscosity (Bear, 1979). To simulate the salt dome flow problem the following equations have to be solved:

\[
v = -\frac{k}{\varepsilon \mu} \cdot (\nabla \rho + \rho g \nabla z)
\]  
(1)

\[
\rho S \frac{\partial \rho}{\partial t} + \varepsilon \frac{\partial \rho}{\partial t} \frac{\partial C_m}{\partial t} + \nabla \cdot (\varepsilon \rho v) = 0
\]  
(2)

\[
\varepsilon \rho \frac{\partial C_m}{\partial t} + \varepsilon \rho v \cdot \nabla C_m = \nabla \cdot (\varepsilon \rho D \nabla C_m)
\]  
(3)

\[
D = D_m I + (\alpha_L - \alpha_T) v v / \|v\| + \alpha_T \|v\| I
\]  
(4)

\[
\rho = \rho(P, C_m)
\]  
(5)

\[
\mu = \mu(P, C_m)
\]  
(6)

where: \(P\) fluid pressure [M/LT²], \(v\) fluid velocity [L/T], \(S\) specific pressure storativity for a rigid solid matrix [(M/LT²)⁻¹], \(\varepsilon\) porosity [-], \(k\)
permeability tensor \( [L^2] \), \( g \) gravity acceleration \( [L/T^2] \), \( \rho \) fluid density \( [M/L^3] \), \( \mu \) fluid dynamic viscosity \( [M/LT] \), \( C_m \) solute mass fraction [-], \( \alpha_L \), \( \alpha_T \) longitudinal and transverse coefficient of mechanical dispersion \([L]\), \( D_m \) pore water diffusion coefficient \([L^2/T]\), \( I \) unit tensor.

As Kolditz et al. (1997) stated in their paper, the success of a numerical solution for variable density flow problems is essentially dependent on evaluating Darcy fluxes for a given discretization. To solve this problem, we use the mixed hybrid finite element approximation (Chavent and Roberts, 1991; Mosé et al., 1994) which is a good method to solve the groundwater flow problem: this approximation gives a velocity throughout the field and the normal component of the velocity is continuous across the inter-element boundaries. Moreover, for this kind of problem, it is useful to build stream functions. With the mixed formulation, the velocity is defined with the help of Raviart Thomas basis functions and therefore a simple integration over the element gives the corresponding streamlines.

Operator and time splitting offer the possibility to adapt an accurate numerical technique for each kind of partial differential equation and to distinguish different boundary conditions for the convective and dispersive transport. Therefore, we split equation (3) as follows:

\[
\varepsilon \rho \frac{C_m^{n+1} - C_m^{n}}{\Delta t} + \frac{C_m^{ad,n+1} - C_m^{n}}{\Delta t} + \varepsilon \rho \nabla C_m = \nabla . (\varepsilon \rho D_m \nabla C_m) + \varepsilon \rho \nabla C_m
\]

(7)

where \( C_m^{ad,n+1} \) is the mass fraction after convection for time step \( n+1 \) calculated by:

\[
\varepsilon \rho \frac{C_m^{ad,n+1} - C_m^{n}}{\Delta t} = -\varepsilon \rho \nabla C_m
\]

(8)

for the convective transport. Discontinuous finite elements coupled with a slope limiting technique is used to solve equation (8) (Siegel et al., 1997).

For the dispersive term of equation (7), we write:

\[
\rho \frac{\partial C_m}{\partial t} = \nabla . (\rho D_m \nabla C_m)
\]

(9)

or, if we neglect the density variation,
The relation between density and mass fraction can be introduced in equation (9). If we have \( \rho = a + bC_m \), equation (9) becomes the following non-linear dispersion equation:

\[
\frac{\partial (\rho^2)}{\partial t} = \nabla \cdot (\mathbf{D} \nabla (\rho^2))
\]  

(11)

The resolution of this last equation can be performed in the same way as (10) if we introduce a new variable \( \chi = \rho^2 \). Equations (10) and (11) are solved by mixed hybrid finite element.

Because of the operator splitting technique, a constant concentration boundary condition can be prescribed for advection (for discontinuous finite elements, concentrations are prescribed at the corner inside the element) and/or dispersion (for mixed finite elements concentrations are prescribed at the element edges). Two kinds of discretization can be applied. The concentrations at the edges (boundary condition for the dispersion term) and the corresponding interior nodes (boundary conditions for the advection term) are imposed. This corresponds to a finite element (FE) type boundary condition discretization. The concentrations at the edge and the four nodes of the corresponding cell are imposed. In this case, we impose concentration throughout the cell, which corresponds to a finite difference (FD) type boundary condition discretization.

3 The salt dome test case

It is a steady state flow and transport problem based on the nuclear waste disposal site at Gorleben, Germany. The groundwater flow is strongly coupled to solute transport since density variations in this example are large (20%). Geometry, parameters and boundary conditions for the problem can be found in numerous papers (Herbert et al., 1988; Konikow et al., 1997 among others).

In the case of pure hydrodynamic dispersion, brine is transported by advection and hydrodynamic dispersion \( (\alpha_L = 20 \text{ m}, \alpha_T = 2 \text{ m and } D_m = 0 \text{ m}^2 \text{ s}^{-1}) \). The final report (OECD, 1988) presents results of different numerical models. These results showed good agreement in that the steady state flow field has a large recirculation in the bottom region. However, there were considerable differences in the final salt distribution (Konikow et al. 1997). The velocity field for the two kinds of boundary condition discretization (FE or FD) showed good agreement in that the steady state flow field has a large recirculation in the bottom region for
the computation made with TVDV-2D. However, there are differences in the final salt distribution. For FD discretization type, we observe that the final salt mass in the system is greater than in the first case. Our results (figure 1) are different from Oldenburg and Pruess (1995). They obtain a final solute distribution pattern that is a swept forward type and suggested that steady state is reached after 100 years. By looking at mass fraction over time at different locations, we found that steady state is reached only after 1000 years. Moreover, we compare the distributions of concentration over the domain at $t = 1000$ years and at $t = 1800$ years which show no significant differences.

For the HYDROCOIN problem, the only source of salt should be from releases by lateral dispersion across the top of salt dome. To simulate this boundary condition, Konikow et al. (1997) suggest extending the domain by adding another row of cells between $x = 300$ m and $x = 600$ m below the previous bottom. In these cells, the concentration imposed is identical to the salt dome. To avoid the advective transport process, the hydraulic conductivity assigned to these cells is much lower than in the active flow field. However, by adding new cells of the same size, the salt flux is dependent on the width of these cells. In our calculation, prescribed concentrations are imposed only at the edges just for dispersion only. Velocity vectors and brine contours obtained with TVDV-2D do not agree with Konikow et al. (1997) results. We find that the same process occurs just as the first case with recirculation in the lower region transporting the dense brine to occupy the entire lower portion of the domain.

The same problem using non-linear dispersion equation (11) has been simulated. Similar results to those obtained by solving the linear dispersion equation (10) were obtained in both cases.

We simulate the salt dome problem with realistic dispersion and diffusion coefficients as follows: $\alpha_t = 0.5$ [m], $\alpha_r = 0.01$ [m], $D_m = 5 \times 10^{10}$ [m$^2$ s$^{-1}$]. We performed three simulations: for the two first, salt is released by advection and dispersion from the constant concentration boundary with a FD (figure 2) and a FE (figure 3) discretization. In the third simulation (figure 4), the salt is released from constant concentration boundary only by dispersion. The total salt mass in the system is greater when the salt is released by advection and dispersion. We can see moreover, that with the finite differences type boundary condition discretization, recirculations are more important and the saltwater-freshwater interface is closer to the left hand side of the domain than with the two other cases. In all cases, recirculation are developed in the lower part of the domain. When the dispersion tensor became small,
recirculations was less pronounced. The saltwater-freshwater interface position and the extent of recirculations do not depend only on the magnitude of dispersion or diffusion, but also on the boundary condition discretization type.

4 Conclusion

The simulations of the salt dome flow problem lead to the following conclusions.
1. Transport equation when the density variations are large is the same than with a tracer. A study of linear dispersion equation and non-linear dispersion equation has been done. It shows that the two approaches are very close.
2. The TVDV-2D code uses robust numerical methods well adapted for density driven flow. The code is also very flexible in boundary condition discretization (FD type, FE type, constant concentration for advection and/or dispersion).
3. As already mentioned by several authors, the salt dome problem is difficult to solve. For each parameter set, the flow field show recirculation cells. These recirculations at x < 300 m vanishes for more physical parameters, which were surprisingly never studied. But they still exist at x > 600 m. For our code, they are less important than recirculations found in prior works. As a consequence, the final concentration distribution is different.
4. Steady state solution is reached after 1000 years.
5. The boundary condition (dispersion - convection or only dispersion) and its discretization (FE or FD type) affect the final results. With TVDV-2D, differences in flow and concentration distribution have been found depending on the boundary conditions.
6. Actually, each numerical method (FD or FE type) solves another problem. Due to the sensitivity of strongly coupled transport to initial and boundary conditions, the different results found in the literature are not surprising and does not mean that one code is more accurate than another. When the dispersive flux is important compared to the grid size and the convective transport, these differences remain small.
References


Figure 1: Flow field vectors and salt contours
\[ D_m = 5 \times 10^{-8} \text{ m}^2 \text{ s}^{-1} \text{ and } t = 1000 \text{ years}. \]

Figure 2: Flow field vectors and salt contours for FD type boundary conditions.

Figure 3: Flow field vectors and salt contours for FE type boundary conditions.

Figure 4: Flow field vectors and salt contours for prescribed dispersive concentration only.