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Modelling of dual porosity media: comparison of different techniques and evaluation of the impact on plume transport simulations

S. BROUYÈRE*, A. DASSARGUES

Laboratoires de Géologie de l'Ingénieur, d'Hydrogéologie et de Prospection Géophysique (L.G.I.H.), University of Liège Bat. B19, B-4000 Liège, Belgium

e-mail: sbrouyer@lgih.ulg.ac.be

R. THERRIEN

Groupe de Recherche In Situ, Département de Géologie et Génie Géologique, Université Laval, Sainte-Foy, Québec G1K 7P4, Canada

E. A. SUDICKY

Department of Earth Sciences, University of Waterloo, Waterloo N2L 3G1, Canada

Abstract The dual porosity concept for a porous medium is based on the presence of regions of immobile water in contact with mobile water. The immobile water, which can be considered as a separate phase, undergoes solute exchange with the mobile water via molecular diffusion. Although field experiments have shown that the dual porosity effect often occurs, this concept is rarely considered in mathematical models used for interpretation. Neglecting the dual porosity effect can lead to erroneous estimation of the hydrodispersive properties. Here, we test and compare two numerical models that incorporate the dual porosity approach with different numerical solutions. We present simulations for a quasi three-dimensional test case consisting of a radially converging flow tracer test in a dual porosity aquifer. Conclusions are drawn on the influence of the dual porosity process on the shape of the breakthrough curves using a parameter sensitivity analysis. Simulations also show how the calibrated transport parameter values are influenced by either neglecting, or taking into account, the dual porosity concept.

INTRODUCTION

Any products dissolved in groundwater migrate by advection and mechanical dispersion. They can also be delayed or definitely trapped, resulting in a longer recorded transit time, a retardation and an attenuation which is noticeable on the measured breakthrough curves. Retardation effects can be classified into two major categories: (a) chemical retardation which includes all the processes for which a chemical reaction between the solute and the aquifer media is involved (sorption–desorption, cation exchange, chemisorption); and (b) physical retardation, often called the dual porosity effect due to the presence in the aquifer media of zones of more or less stagnant water (dead-end pores, low conductivity lenses, etc.), where solutes can migrate by molecular diffusion processes. In practice, dual porosity concepts can be

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applied to many situations where the fact that the flow velocity distribution departs from the classical Gaussian distribution does not allow use of the advective–dispersive transport equation (ADE). The occurrence of low (or null) velocity zones requires one to conceptually define a separate phase containing immobile water. This is often the case in fissured rocks like chalks, in aggregated soils (macroporous soils), and in very heterogeneous or stratified aquifers. Mathematically, the solute exchange between mobile and stagnant water is often represented with a first-order transfer equation which depends on the concentration difference between the two phases.

In this paper, we present the results obtained with two finite element simulators (SUFT3D and FRAC3DVS) which numerically deal with the dual porosity concept in different ways, applied to a semi-three-dimensional test case consisting of modelling a radially converging flow tracer test. This test is further used for a parameter sensitivity analysis. Conclusions are drawn on the influence of the dual porosity process on the shape of the breakthrough curves. Simulations also show how the calibrated transport parameter values are influenced by considering or neglecting the dual porosity concept. To do this, computed breakthrough curves are re-interpreted using a semi-analytical solution which does not consider the dual porosity concept.

MODELLING DUAL POROSITY

The concept of dual porosity was first introduced by Coats & Smiths (1964). Gallo *et al.* (1996) have compared and summarized different approaches to deal with the dual porosity concept in numerical simulators (finite elements or finite differences).

The mass balance equations for the transport of a solute in subsurface media, and for the immobile water, respectively, can be written as follows :

$$\theta_m \frac{\partial C_m}{\partial t} = -\underline{V} \cdot \underline{\nabla} C_m + \underline{\nabla} \cdot \left(\theta_m \underline{\underline{D}} \cdot \underline{\nabla} C_m\right) - \lambda \theta_m C_m - \alpha\left(C_m - C_{im}\right) + Q\left(C_{in} - C_m\right) \quad (1)$$

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = -\lambda \theta_{im} C_{im} + \alpha\left(C_m - C_{im}\right) \quad (2)$$

In these equations, C_m, C_{im} and C_{in} are the concentrations [M L^{-3}] in the mobile, the immobile water, and an injected fluid through a sink term; θ_m, θ_{im} are the effective and immobile water porosity [–]; $\underline{V}$ is the Darcy flux [L T^{-1}]; $\underline{\underline{D}}$ the hydrodynamic dispersion tensor [L^2 T^{-1}], α the first order transfer coefficient between the mobile and the immobile water [T^{-1}]; λ the linear decay constant [T^{-1}]; and Q the injection/pumping rate [T^{-1}].

Most often, an approximate solution is evaluated over time for equation (2) and substituted in equation (1) before computing the numerical solution to the problem. The dual porosity concentrations are updated at the end of each time step according to the computed transport results.

The differences between the codes mainly concern the way the immobile water concentration is evaluated. In SUFT3D, a semi-analytical solution describes the concentration evolution in the immobile water over a time step (Biver, 1993). In FRAC3DVS, a finite time-differencing scheme similar to that described in Ibaraki & Sudicky (1995) is used. Details of the possibilities and efficiency of both codes can be

found in Therrien & Sudicky (1996) for FRAC3D, and in Carabin & Dassargues (1999) for SUFT3D.

To test the dual porosity concept in SUFT3D, the results were first checked (Brouyère & Dassargues, 1997) with the analytical one-dimensional solution of van Genuchten & Wierenga (1976). The results of SUFT3D and FRAC3DVS were compared on a simple test case consisting of a radially converging flow tracer test. The injection well is located 20 m from a pumping well where a constant flow rate of 10 $m^3 h^{-1}$ is extracted. A unit mass of tracer is injected over one hour. The aquifer has a uniform thickness of 8 m and a conductivity of 5×10^{-4} m s^{-1}. The initial total heads are uniformly taken at 10 m (the aquifer is confined and saturated). The aquifer parameters are representative of a chalky dual porosity aquifer (Hallet, 1998): θ_m = 0.01, α_L = 5 m and α_T = 0.5 m. For the validation test, the first order transfer coefficient (α) was varied from zero to 10^{-5} s^{-1}, θ_{im} being set to 0.30. Small discrepancies were noted due to the different integration methods and mesh refinement used with both codes. As mentioned by Gallo *et al.* (1996), the numerical strategies used to model the dual porosity concept can differ from a stability point of view when α is high. The approaches coded in SUFT3D and FRAC3DVS seem to be very stable, even for transfer coefficients as high as 10^{-5} s^{-1}, which (to our knowledge) can be considered far higher than the upper actual limit for a chalk material.

PARAMETER SENSITIVITY ANALYSIS

Radially converging tracer tests are often used experimentally to define the parameters governing the migration and retardation of a solute in groundwater. If no retardation or capturing effect is involved, all the injected tracer should be recovered at the pumping well. A recovery factor less than unity indicates tracer migration in another direction or a strong delay in the tracer recovery.

Dual porosity effects can have a significant influence on the solute transport and on the recovery factor. The parameter sensitivity analysis described on the same test case (using SUFT3D) illustrates this fact. First, α is varied with θ_{im} kept constant (θ_{im} = 0.20). Then, α is kept constant ($\alpha = 3 \times 10^{-7}$ s^{-1}) and θ_{im} varied from 0 to 0.30. The resulting breakthrough curves are shown in Figs 1 and 2. The concentration peak amplitude depends mainly on the α value. When α is increased, the peak is lower and is reached earlier. The first arrival of the tracer does not seem to be affected by the magnitude of α. These effects are easy to explain if we note the similarity between the first order transfer coefficient α and a linear decay constant (λ). At early times, C_{im} is negligible compared to C_m in equation (2), which in this case is similar to a degradation equation. From a practical point of view, this means that even with a numerical code that cannot model dual porosity effects, it is possible to evaluate the first-order transfer coefficient, provided that a linear degradation is proposed. Applying a similarity, an "equivalent degradation coefficient" is given by :

$$\lambda_{eq} = \frac{\alpha}{\theta_m} \tag{3}$$

It was tested here with $\alpha/\theta_m = 3 \times 10^{-5}$ s^{-1} equivalent to $\alpha = 3 \times 10^{-7}$ s^{-1} and θ_m = 0.01. The resulting breakthrough curve is very close to the equivalent dual porosity

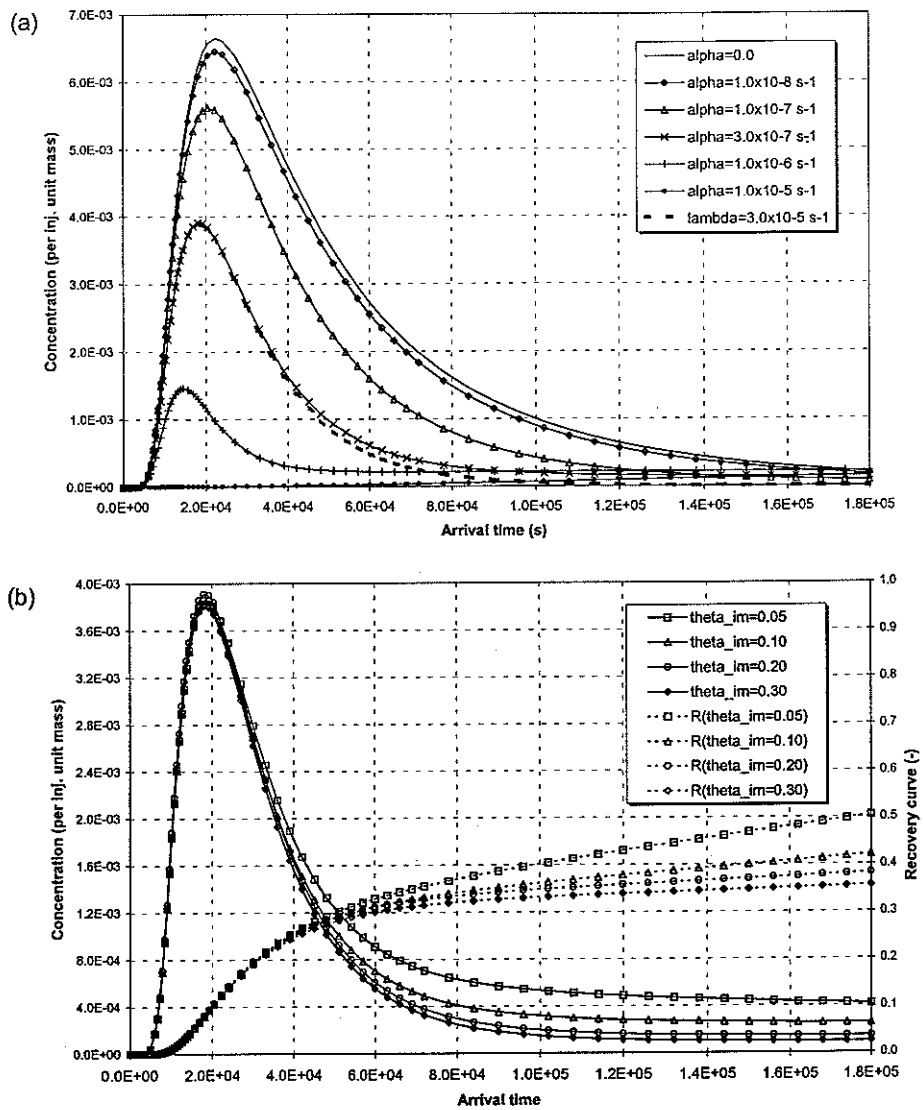

Fig. 1 Influence of (a) the first order transfer coefficient (α), and (b) the immobile water content (θ_{im}) on the shape of the breakthrough curve.

breakthrough curve (Fig. 1(a)) except for later times when the concentration goes to zero, not reproducing the long flat tail resulting from the back diffusion of the solute from immobile water to mobile water. For $\alpha = 10^{-6}$ s^{-1}, a second very flat peak appears on the breakthrough curve. To the limit when α becomes very high (10^{-5} s^{-1}), only a single flat peak is visible, switched to late times. For such high values of α, a new equilibrium is reached and a lumped advection–dispersion could be used with a modified effective porosity equal to the total porosity and a modified dispersion term accounting for the dispersion effect due to the high transfer rate between mobile and immobile water.

As shown in Fig. 1(b), θ_{im} does not have a strong influence on the concentration peak amplitude or position (on the time axis). But the influence of θ_{im} is clearly visible on late arrivals: the higher θ_{im}, the lower the concentrations at the pumping well. In equation (2), θ_{im} is the inertial coefficient multiplying the time derivative of C_{im}. When θ_{im} is high, the time evolution of C_{im} is low and C_{im} does not rise quickly. After the peak, the concentration in the mobile water can decrease quickly, to a low value close to the concentration in immobile water. If θ_{im} is low, C_{im} rises more rapidly, reaching a higher "background" level that boosts the concentration in the mobile water after the peak, thanks to a high level back-diffusion of solute.

The slope of the recovery curve is clearly related to the amplitude of θ_{im}: the higher θ_{im}, the lower the slope. Recovery curves could thus provide a good possible means for assessing θ_{im} independently from the other parameters. From a practical point of view, a low observed recovery factor can be easily explained by a dual porosity effect. If the test medium is characterized by a high θ_{im}, the breakthrough curve tail can be very long with a low concentration. In that case, most of the tracer is recovered at a concentration lower than detection limit.

INFLUENCE OF THE DUAL POROSITY CONCEPT ON THE EVALUATION OF OTHER TRANSPORT PARAMETERS

Dual porosity effects are rarely considered, mainly because very few of the usual commercial codes include this concept. Evaluation of the transport parameters (most often the effective porosity and longitudinal dispersivity) is often based on a trial-and-error visual fitting of the computed breakthrough curve to the measured one. As shown in the test case, the parameters related to the dual porosity effect (the first-order transfer coefficient and immobile water porosity) have a significant influence on the shape of the breakthrough curve. If they are not considered in the calibration, errors can result in the assessment of the other transport parameters.

To check it, some of the breakthrough curves obtained with the code SUFT3D were re-interpreted without considering any dual porosity effect. In order to have an objective calibration, a least-squares method was used (rather than a trial-and-error calibration), using the code CATTI (Sauty *et al.*, 1992). The fitting parameters are: the effective porosity (θ_m), the longitudinal dispersivity (α_L) and the recovery factor (R_F). The last parameter had to be used as a fitting parameter because it was impossible to get reliable estimates of θ_m and α_L by considering a unit recovery factor. This is often the case when using analytical solutions.

The transport parameters as fitted with CATTI differ from the actual transport parameters used with SUFT3D without a dual porosity effect. This is because the semi-analytical solution proposed in CATTI supposes that the transverse dispersion is negligible and the injection is modelled with a Dirac-type function. Table 1 summarizes the resulting transport parameters (θ_m, α_L and R_F) as fitted with CATTI, together with the actual parameters used with SUFT3D, for different values of α (θ_{im} is fixed at 0.20). Although further tests could be useful to gain a better idea of the influence, this clearly confirms that neglecting the dual porosity effect can lead to large underestimates of the effective porosity (θ_m) and the longitudinal dispersivity (α_L).

Table 1 Influence of α on the calibrated transport parameters (θ_m, α_L).

	SUFT3D	CATTI	SUFT3D	CATTI	SUFT3D	CATTI
α	0.0	–	3×10^{-7}	–	10^{-6}	–
θ_m	0.01	0.01428	0.01	0.00876	0.01	0.00639
α_L	5.0	5.89	5.0	3.54	5.0	2.85
R_F	1.0	0.973	1.0	0.347	1.0	0.088

CONCLUSIONS

Two finite element simulators using different numerical approaches were compared. A quasi three-dimensional test case is proposed to check the results and efficiency of the simulators with a practical example consisting of a radially converging flow tracer test. The test case could be used further, with analytical solutions, as a reference test to validate and check the coding of the dual porosity concept in other numerical codes.

Sensitivity analysis of the dual porosity provided interesting conclusions: the first-order transfer coefficient has a significant impact on the amplitude of the breakthrough concentration peak at the pumping well. The immobile water porosity does not affect the peak amplitude much but has a major effect on the tail of the breakthrough; a very long tail is produced at low concentrations with a high immobile water porosity, cf. a higher, quickly descending tail with a low immobile water porosity. It was also shown that an equivalent degradation coefficient can be used to estimate the first order transfer coefficient.

Tests of the calibration without considering the dual porosity effect have proved that neglecting the dual porosity effect can lead to underestimation of θ_m and α_L by as much as 50%. More numerical experiments are needed to define accurately the influence on the interpretation.

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