TRANSPORT EQUATION FOR THE CONCENTRATION GRADIENT

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Summary The organization and dynamic of the concentration in the heterogeneous porous media are key physical factors driving the chemical reactivity. At equilibrium, the chemical reactivity depends not only on the concentration distribution but also on concentration gradients for a simple precipitation. We derive the transport equation for concentration gradient and set up an adapted diffusion velocity method to approximate them numerically. The numerical results give optimal predictions of the chemical reactivity.

INTRODUCTION

A precipitate P dissolves yielding two solute species A and B, $P \Leftrightarrow A + B$. Solute concentrations c_A and c_B are related through the equilibrium constant $K = c_A c_B$. The reactive rate r between the two species A and B is given by :

$$r = \frac{2K}{((\delta c)^2 + K)^{3/2}} \nabla(\delta c) D \nabla(\delta c) \quad \text{with} \quad \delta c = c_A - c_B \tag{1}$$

Reactivity does not depend only on the concentration distribution but also on the local diffusive dynamic of concentration mixing [Le Borgne et al., 2010]. Concentration gradients follow complex spatial and temporal dynamics as they are created by velocity gradients through elongation and shear stress of the mixing fronts and dissipated by diffusion [Le Borgne et al., 2015]. Numerical methods should give accurate approximations of both concentration distributions and concentration gradients. The transport equation for concentration gradients is derived and solved with a particle method based on a diffusion velocity scheme [Beaudoin et al., 2003]. The particle methods are frequently used to solve the transport equation in porous and fractured media [Beaudoin et al., 2013] [Robinet et al., 2013]. When transport by advection largely dominates dispersion and diffusion processes, the particle methods offer a relevant alternative to Eulerian methods [Zhang et al., 2007]. Furthermore, particle methods can handle a large panel of inert as well as chemical and biological particle types [Tartakovsky et al., 2007].

TRANSPORT EQUATION OF CONCENTRATION GRADIENTS

The transport equation of concentration gradient $\nabla \delta c$ i obtained by applying ∇ to the transport equation :

$$\nabla \left(\frac{\partial \delta c}{\partial t} - \nabla \cdot (D\mathbf{g}) + \nabla \cdot (\mathbf{u}\delta c) \right) = 0 \quad \text{with} \quad \mathbf{g} = \nabla \delta c \tag{2}$$

where D is the diffusion coefficient, g the concentration gradient and u the flow velocity. Using the properties of vector operators and the assumptions of incompressible and irrotational flow, the previous equation becomes :

$$\frac{\partial \mathbf{g}}{\partial t} - \nabla \cdot (\nabla (D\mathbf{g})) + (\mathbf{g} \cdot \nabla)\mathbf{u} + \nabla \cdot (\mathbf{u} \otimes \mathbf{g}) = 0 \tag{3}$$

The last step consists in writing the diffusion term of equation (3) as an advection term by means of the diffusion velocity :

$$\frac{\partial \mathbf{g}}{\partial t} + \nabla \cdot ((\mathbf{u_d} + \mathbf{u}) \otimes \mathbf{g}) + (\mathbf{g} \cdot \nabla)\mathbf{u} = 0 \quad \text{with} \quad \mathbf{u_d} \otimes \mathbf{g} = -\nabla (D\mathbf{g}) \tag{4}$$

where u_d is the diffusion velocity. The transport equation of g (Eq. 3) is then transformed in a purely convective equation with a source term (Eq. 4). The expression of u_d is derived by means of a simple identification between equations (3) and (4).

NUMERICAL RESULTS

The transport of a concentration difference δc between two species is studied in a 2D heterogeneous flow field, see Figure 1. The porous medium is defined by a rectangle with the dimensions Lx = 2048 m and Ly = 512 m. The mean flow direction is the x axis. The permeability field K, assumed isotropic and heterogeneous, is characterized by a stationary log-normal probability distribution $Y = ln(K)$, defined by a zero mean and a covariance function given by $C(r) = \sigma^2 exp(-|r|/\lambda)$ where σ^2 and λ are the variance and the correlation length of Y. σ^2 and λ are fixed to 4 and 10 m. The classical laws governing the steady flow in a porous medium are mass conservation and Darcy law, $u = -K\nabla P$ and $\nabla \cdot u = 0$ with P the

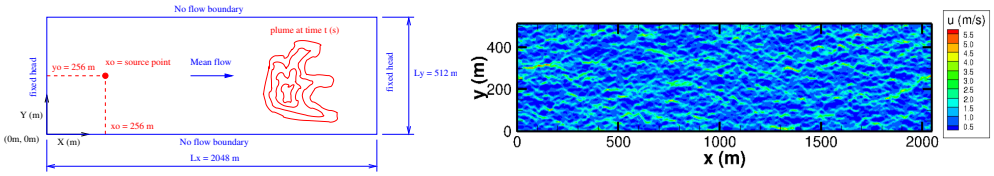

Figure 1: Scheme of problem considered (left) and horizontal component of the flow velocity (right).

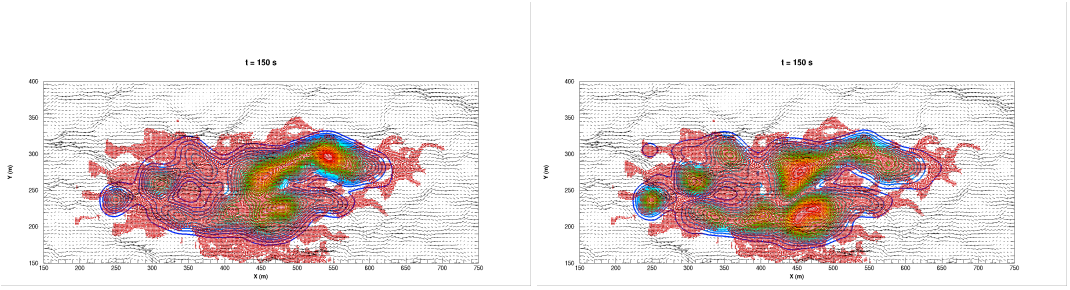

Figure 2: Concentration difference δc (left, colored contour lines) and its gradient norm $|g|$ (right, colored contour lines) with the set of numerical particles (full red circles) at time t = 150 seconds. The black arrows show the flow field.

hydraulic head. Boundary conditions are homogeneous Neumann on upper and lower sides, and Dirichlet P = 0 on left side and $P = Lx$ on right side. To characterize the mass transport, the Peclet number is defined by $Pe = \lambda|u|/D$. The norm of the mean flow velocity $|u|$ is equal to 1 m/s. Thus the Peclet number Pe is equal to 10000 for a diffusion coefficient D = 0.001 m^2/s. At the initial time, the concentration difference δc is injected at the source point Xo = (256 m, 256 m). The numerical simulation is stopped at time t = 150 seconds. The set of numerical particles is initialized by using a gaussian function. Figure 2 shows the concentration difference δc (left) and its gradient norm $|g|$ (right) with the set of numerical particles at time t = 150 seconds. We can observe that the negative values do not appear on the field of δc. Thus the chemical mechanisms can be simulated efficiently. The fields of δc and $|g|$ follow the flow. The zones of high values and low values are the same for the two quantities. The gradient particle method seems to simulate correctly the effects of the heterogeneous flow on the transport of the concentration, mixing and spreading. These two mechanisms are important for evaluating the impact of the heterogeneous flow on the chemical reactivity. These first results, obtained from the context of modelling groundwater flow and mass transport, allow to show how the gradient particle method can be used for simulating the reactive transport in high heterogeneous porous media.

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