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Analytic Solution of Pseudocolloid Migration in Fractured Rock

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A form of colloid migration that can enhance or retard the migration of a dissolved contaminant in ground water is the sorption of the contaminant on the moving colloidal particulate to form pseudocolloids. In this paper we develop analytical solutions for the interactive migration of radioactive species dissolved in ground water and sorbed as pseudocolloids.

The solute and pseudocolloids are assumed to undergo advection and dispersion in a one-dimensional flow field in planar fractures in porous rock. Interaction between pseudocolloid and dissolved species is described by equilibrium sorption. Sorbed species on the pseudocolloids undergo radioactive decay, and pseudocolloids can sorb on fracture surfaces and sediments. Filtration is neglected. The solute can decay and sorb on pseudocolloids, on the fracture surfaces, and on sediments and can diffuse into the porous rock matrix.

The mass balance for the pseudocolloid, per unit volume of fracture, is

$$\epsilon_1 \xi_1 \frac{\partial C_1(x,t)}{\partial t} + \epsilon_1 \xi_1 v_1 \frac{\partial C_1(x,t)}{\partial x} + \epsilon_1 S_1(x,t) + \epsilon_1 S_2(x,t) - \epsilon_1 \xi_1 D_1 \frac{\partial^2 C_1(x,t)}{\partial x^2} + \epsilon_1 \xi_1 \lambda C_1 = 0, \quad x > 0, t > 0 \quad (1)$$

where $C_1(x,t)$ is the amount of species sorbed on the colloid per unit volume of solid colloid, v_1 is the colloid pore velocity, D_1 is the colloid dispersion coefficient, λ is the decay constant, ϵ_1 is the porosity within the fracture, ξ_1 is the constant volume fraction of pseudocolloids in fracture liquid, $\epsilon_1 S_1(x,t)$ is the rate of sorption to stationary solid, $\epsilon_1 S_2(x,t)$ is the rate of desorption from the pseudocolloid.

For the same species as solute in liquid in the fracture

$$\epsilon_1 \frac{\partial C_2(x,t)}{\partial t} + \epsilon_1 v_2 \frac{\partial C_2(x,t)}{\partial x} - \epsilon_1 S_2(x,t) + \epsilon_1 S_3(x,t) - \epsilon_1 D_2 \frac{\partial^2 C_2(x,t)}{\partial x^2} + \epsilon_1 \lambda C_2 + \frac{q(x,t)}{b} = 0, \quad x > 0, \quad t > 0 \quad (2)$$

where $C_2(x,t)$ is the solute concentration in the fracture liquid, v_2 is the solute pore velocity, $\epsilon_1 S_3(x,t)$ is the rate of solute sorption on stationary fracture solids, b is the fracture half-width, and q(x,t) is the diffusive solute flux into the rock matrix, given by

$$q(x,t) = -\epsilon_p D_p \frac{\partial N(x,y,t)}{\partial y} \bigg|_{y=b}, \qquad x > 0, \quad t > 0$$
(3)

 ϵ_p is the rock porosity, D_p is the solute diffusion coefficient in rock, and N(x, y, t) is the solute concentration in pore water in the rock.

For solute species sorbed on stationary fracture solids

$$(1 - \epsilon_1) \frac{\partial C_3(x, t)}{\partial t} - \epsilon_1 S_3 + (1 - \epsilon_1) \lambda C_3(x, t) = 0, \qquad x > 0, \qquad t > 0$$

$$(4)$$

where $C_3(x,t)$ is the concentration of sorbed solute species..

For species sorbed as pseudocolloids on the stationary fracture solids

$$(1 - \epsilon_1)\xi_2 \frac{\partial C_1(\mathbf{x}, t)}{\partial t} - \epsilon_1 S_1(\mathbf{x}, t) + (1 - \epsilon_1)\xi_2 \lambda C_1(\mathbf{x}, t) = 0, \qquad \mathbf{x} > 0, \qquad t > 0$$
 (5)

where ξ_2 is the constant volume fraction of the sorbed colloid per unit volume of the stationary fracture solid

Inside the rock matrix

$$R_{p} \frac{\partial N(x,t)}{\partial t} - D_{p} \frac{\partial^{2} N(x,t)}{\partial y^{2}} + R_{p} \lambda N(x,t) = 0, \quad x > 0, \quad t > 0, \quad y > 0$$
 (6)

where R_p is the solute retardation coefficient in the rock matrix.

We assume linear sorption equilibrium between the solute species in the fracture liquid and the same species sorbed on the colloid. Both the solute species and the colloids in the fracture liquid are assumed to undergo linear sorption equilibrium with the fracture solids

$$K_{d_1} = \frac{C_1(x,t)}{C_2(x,t)}, \qquad K_{d_2} = \frac{\xi_2}{\xi_1}, \qquad K_{d_3} = \frac{C_3(x,t)}{C_2(x,t)}$$
 (7)

From eq. (1)-(5), we can obtain the equation for c_1 in terms of the effective retardation factor R, dispersion coefficient D, and velocity v.

$$R\frac{\partial C_1(x,t)}{\partial t} + v\frac{\partial C_1(x,t)}{\partial x} - D\frac{\partial^2 C_1(x,t)}{\partial x^2} + R\lambda C_1(x,t) + \frac{q(x,t)}{\epsilon_1 b} = 0, \quad x > 0, \quad t > 0$$
 (8)

where

$$R = \left[\xi_1 \left(1 + \frac{1 - \epsilon_1}{\epsilon_1} K_{d_2}\right)\right] + \left[1 + \frac{1 - \epsilon_1}{\epsilon_1} K_{d_3}\right] \frac{1}{K_{d_1}}$$

$$\tag{9}$$

$$v = v_1 \left(\xi_1 + \frac{v_2}{K_{d_1} v_1} \right) \tag{10}$$

$$D = D_1 \left(\xi_1 + \frac{D_2}{D_1 K_{d_1}} \right) \tag{11}$$

The initial and boundary conditions are

$$N(x, \infty, t) = 0, \qquad x > 0, \quad t > 0 \tag{12}$$

$$N(x,b,t) = \frac{1}{K_{d}}C_1(x,t), \qquad x > 0, \quad t > 0$$
 (13)

$$N(x, y, 0) = 0, x > 0, y > 0 (14)$$

$$C_1(0,t) = K_{d_1}C_{o_1}, t > 0$$
 (15)

$$C_1(\infty, t) = 0, \qquad t > 0 \tag{16}$$

$$C_1(x,0) = 0, x > 0 (17)$$

where C_o is the inlet solute concentration.

The solution is

$$C_{1} = \frac{2K_{d_{1}}C_{o}}{\sqrt{\pi}} \int_{\frac{\pi}{2}\sqrt{R/Dt}}^{\infty} \exp\left\{-\frac{\sqrt{v^{2}+4R\lambda D}-v}{2D}x\right\} \operatorname{erfc}\left[\frac{x^{2}\epsilon_{p}\sqrt{D_{p}}R_{p}}{8Db\epsilon_{1}\eta^{2}\sqrt{t-\frac{Rx^{2}}{4D\eta^{2}}}}\right] \exp\left[-\left(\eta-\frac{xv}{4D\eta}\right)^{2}\right] d\eta$$

$$x > 0, t > 0 \tag{18}$$

In Figure 1, we show the concentration profiles of species as solute and pseudocolloid, for assumed parameters and for a step release. Matrix diffusion of the solute, together with dispersion in fracture flow, result in a monotonic decrease in the concentrations of solute and pseudocolloids, approaching zero concentration at the front. Solute and pseudocolloid remain in constant ratio within the fracture liquid.

In a separate publication we will present a similar analysis of coupled transport of colloids and solute, with solubility equilibrium between the colloid and solute.

Figure 1. Relative Concentration of Pseudocolloid and Solute, Fracture Flow and Matrix Diffusion of Solute

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