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# Reactive silica transport in fractured porous media: Analytical solution for a single fracture

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ABSTRACT

A general analytical solution is derived by using the Laplace transformation to describe transient reactive silica transport in a conceptualized 2-D system involving a single fracture embedded in an impervious host rock matrix. This solution differs from previous analyses in that it takes into account both hydrodynamic dispersion and advection of silica transport along the fracture, and hence takes the form of an infinite integral. Several illustrative calculations are undertaken to confirm that neglecting the dispersion term may lead to erroneous silica distribution along the fracture and within the host matrix, and the error becomes severe with a smaller rate of fluid flow in the fracture. The longitudinal dispersion is negligible only at steady state or when the flow rate in the fracture is higher. The analytical solution can serve as a benchmark to validate numerical models that simulate reactive mass transport in fractured porous media.

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## 1. Introduction

It is well known that fractures play an important role in controlling fluid flow, heat transfer and contaminant transport, due to their commonly higher permeability compared with that of the host media. If the fluid flow rate is assumed to be constant in a single fracture or a set of parallel fractures embedded in an impervious host rock, then analytical solutions are derivable to define non-reactive solute transport (e.g., Tang et al., 1981; Sudicky and Frind, 1982; Ling et al., 2002; West et al., 2004) and heat transport (e.g., Bodvarsson, 1969; Gringarten et al., 1975; Lowell, 1976; Yang et al., 1998). More recently, Graf and Simmons (2009) considered variable-density flow and solute transport in a vertical fracture by adding a density-driven flow component to the standard Tang et al. (1981) analytical solution.

Quartz is most common in the upper crust, and its precipitation and dissolution have drawn constant attention due to the essential role in altering crustal porosity and permeability and hence impacting the dynamics of fluid flow and contaminant transport as well as the thermal regime (e.g., Fournier, 1983, 1985; Brady and Walther, 1989; Lowell et al., 1993; Tester et al., 1994; Dove, 1999). Silica (an aqueous form of quartz) and its transport in a single fracture have been addressed analytically by Steefel and Lichtner (1998) to verify their numerical scheme that aims at modeling the reaction front geometry in a discrete fracture–matrix system. The same analytical solution has also been employed recently by Graf and Therrien (2007) to validate their 3-D numerical model that simulates coupled fluid flow, heat and single-species reactive mass transport in fractured porous media. In deriving the analytical solution, however, the previous studies failed to take into account molecular diffusion and mechanical dispersion of silica transport in the fracture, which is problematic especially for the case with low flow rate in the fracture.

The purpose of this paper is to derive a general analytical solution subject to all diffusive and dispersive processes for accurate determination of silica transport along a single fracture and within the host matrix. The present approach differs from previous solutions (e.g., Sudicky and Frind, 1982) since the rate coefficients are unique for the matrix and fracture. Several case calculations are presented to illustrate the negative impact resulting from neglecting such a longitudinal dispersion term in the fracture. The paper also investigates how a variation in fluid velocity influences the silica distribution and under what conditions the longitudinal dispersion becomes negligible. The analytical solution developed here is particularly useful in evaluating the accuracy of numerical models of reactive mass transport in fractured porous media, and is also helpful in obtaining a first-order estimate of the transport solution prior to numerical modeling.

## 2. Conceptualized physicochemical system and governing equations

A thin rigid fracture is embedded in a porous matrix, as illustrated in Fig. 1. Aqueous silica is assumed to be the only species that undergoes chemical interactions (dissolution/precipitation) with the rock matrix. The entire domain is saturated with silica-saturated

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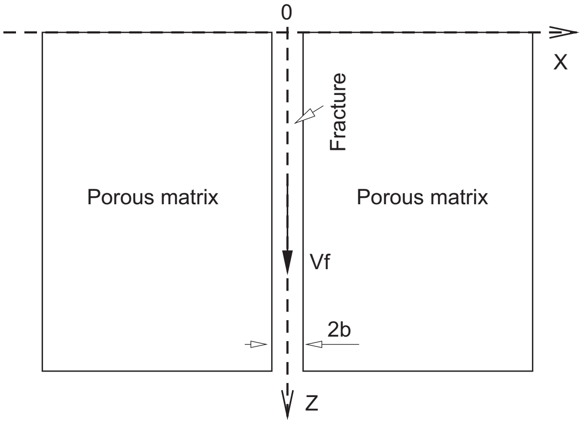

**Fig. 1.** A 2-D conceptualized fracture–matrix system.

fluid and is in thermodynamic equilibrium. Silica-free freshwater enters the fracture inlet on the top and dilutes the silica-saturated fluid in the fracture and the host matrix, resulting in a drop of silica concentration in the domain. Heat transport is not considered in this study, but a constant background temperature is imposed.

It is assumed that the silica-free freshwater velocity in the fracture $v_f$ is constant, the width of the fracture $2b$ is much smaller than its length so that the variation in silica concentration across the fracture's aperture is negligible, the permeability and porosity of the porous matrix are very low so that silica transport within the matrix is mainly by molecular diffusion, and that silica transport along the fracture by molecular diffusion, mechanical dispersion and advection is much faster than transport within the matrix. It is further assumed that the material properties (i.e., matrix porosity, permeability, fracture aperture, and mineral surface areas) are constant. These assumptions provide the basis for a 1-D representation of silica transport along the fracture itself and for taking the direction of silica flux in the porous matrix to be perpendicular to the facture. This results in the simplification of the basically 2-D system to two orthogonal, coupled 1-D systems.

The quartz–water reaction defined in the above physiochemical system can be described as

$$SiO_{2(s)}+2H_2O_{(aq)} \Leftrightarrow H_4SiO_{4(aq)}, \tag{1}$$

where $SiO_{2(s)}$is solid quartz, and $H_4SiO_{4(aq)}$ is aqueous silica. Let $C_m'$and $C_f'$ represent the molal concentration of silica in the host matrix and fracture, respectively, and organize them in the form

$$C'_m = C_m + K_{eq} \quad \text{and} \quad C'_f = C_f + K_{eq}, \tag{2}$$

where $K_{eq}$ is the quartz solubility (or equilibrium constant) of the water-rock reaction stated in Eq. (1), and the new variables $C_m$ and $C_f$ represent the 'degree of disequilibrium' of the silica in solution.

In their previous studies, Steefel and Lichtner (1998) and Graf and Therrien (2007) reported the governing equations of this transport problem using the new variables, but for a simplified case without considering hydrodynamic dispersion of silica transport in the fracture. When taking into account this dispersion term, $C_m$ and $C_f$ satisfy the following governing equations, modified from the formulation of Graf and Therrien (2007)

$$\frac{\partial C_m}{\partial t} - D_m \frac{\partial^2 C_m}{\partial x^2} + \frac{\phi_{qz} k_+^0 A_{qz}}{\phi K_{eq}} C_m = 0, \quad b \le x \le \infty \tag{3}$$

and

$$\frac{\partial C_f}{\partial t} - D_f \frac{\partial^2 C_f}{\partial z^2} + v_f \frac{\partial C_f}{\partial z} + \frac{\phi_{qz} k_+^0 A_{qz}^f}{K_{eq}} C_f - \frac{\phi D_m}{b} \frac{\partial C_m}{\partial x}\Big|_{x=b} = 0, \quad 0 \le z \le \infty \tag{4}$$

subject to the boundary conditions

$$C_f(z,t)|_{z=0} = C_{f0}, \tag{5}$$

$$C_m(x,z,t)|_{x=\infty} = 0, \tag{6}$$

$$C_m(x,z,t)|_{x=b} = C_f(z,t), \tag{7}$$

and the initial conditions

$$C_f(z,t)|_{t=0} = 0, \quad C_m(x,z,t)|_{t=0} = 0, \tag{8}$$

where $\phi$ is the matrix porosity, $\phi_{qz}$ is the quartz volume fraction ($\phi_{qz}$=$1-\phi$), $k_+^0$ is the dissolution rate constant, $A_{qz}$ is the specific quartz surface area in the matrix, $A_{qz}^f$ is the specific quartz surface area in the fracture, $D_m = \tau D_w$ is the effective diffusion coefficient in the matrix ($\tau$ is the tortuosity, and $D_w$ is the diffusion coefficient in water), $D_f = \alpha_l v_f + D_w$ is the hydrodynamic dispersion coefficient in the fracture ($\alpha_l$ is the longitudinal dispersivity), and $t$ is the time.

Let $\lambda_m = \phi_{qz} k_+^0 A_{qz}/\phi K_{eq}$ and $\lambda_f = \phi_{qz} k_+^0 A_{qz}^f/K_{eq}$ represent the reaction rate constants in the rock matrix and in the fracture, respectively, and $D'_m = \phi D_m/b$, then the governing Eqs. (3) and (4) become

$$\frac{\partial C_m}{\partial t} - D_m \frac{\partial^2 C_m}{\partial x^2} + \lambda_m C_m = 0 \tag{9}$$

and

$$\frac{\partial C_f}{\partial t} - D_f \frac{\partial^2 C_f}{\partial z^2} + v_f \frac{\partial C_f}{\partial z} + \lambda_f C_f - D'_m \frac{\partial C_m}{\partial x}\Big|_{x=b} = 0. \tag{10}$$

## 3. Analytical solutions

### 3.1. General transient solution

Applying the Laplace transformation to (9) yields

$$(s+\lambda_m)\overline{C_m} = D_m \frac{d^2 \overline{C_m}}{d^2 x}, \tag{11}$$

where $\overline{C_m}$ is the Laplace transformation of $C_m$, defined as

$$\overline{C_m}(x,s) = \int_0^\infty \exp(-st) C_m(x,t)\, dt. \tag{12}$$

The only possible solution for (11) is of the form

$$\overline{C_m} = c_1 \exp[-(S/D_m)^{1/2}(x-b)], \quad (S = s+\lambda_m), \tag{13}$$

where the constant $c_1$ can be obtained by using the boundary condition (7). Thus (13) becomes

$$\overline{C_m} = \overline{C_f} \exp[-d_m S^{1/2}(x-b)], \tag{14}$$

where

$\overline{C_f}$ is the Laplace transformation of $C_f$, and $d_m = (1/D_m)^{1/2}$. (15)

The gradient of $\overline{C_m}$ at the interface $x$=$b$ is

$$\frac{d\overline{C_m}}{dx}\Big|_{x=b} = -d_m S^{1/2} \overline{C_f}. \tag{16}$$

Applying the Laplace transformation to Eq. (10) yields

$$s\overline{C_f} - D_f \frac{d^2 \overline{C_f}}{dz^2} + v_f \frac{d\overline{C_f}}{dz} + \lambda_f \overline{C_f} - D'_m \frac{d\overline{C_m}}{dx}\Big|_{x=b} = 0. \tag{17}$$

Substituting (16) into (17), one has

$$\frac{d^2 \overline{C_f}}{dz^2} - \frac{v_f}{D_f} \frac{d\overline{C_f}}{dz} - \frac{1}{D_f}\left[S + \frac{S^{1/2}}{A} + d\lambda\right]\overline{C_f} = 0, \tag{18}$$

where $A = 1/(D'_m d_m)$, and $d\lambda = \lambda_f - \lambda_m$.

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