

## Solute Transport in Rock Fractures

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### Abstract

This study aims at investigating the relationship between dispersion coefficient ratio to molecular diffusion coefficient ( $D_L/D_m$ ) and Peclet number ( $Pe$ ) for multi-solute system in non-Darcian flow regime. Existing understanding on solute dispersion is primarily derived from one-solute system in Darcian flow regime. We found that solute dispersion in rock fractures can be characterized by the mechanism of both macrodispersion and Taylor dispersion, even for non-Darcian flow domain. For the Darcian flow regime, even different solutes lead to the same  $D_L/D_m$  at same  $Pe$ . However, as the flow becomes non-Darcian, solute with a higher molecular diffusion coefficient result in higher  $D_L/D_m$  at the same  $Pe$  than that with a lower diffusion coefficient.

**key words:** solute transport, Taylor dispersion, macrodispersion, rock fractures

### 1. Introduction

Solute transport in rock fractures is of a great concern for the remediation of contaminated groundwater and for radioactive waste disposal in fractured rocks. Of central importance to understand and predict solute transport in fractured rocks is the relationship between dispersion coefficient and the fluid velocity.

*Keller et al.* [1999] showed a linear relationship between the longitudinal dispersion coefficient  $D_L$  and the average fluid velocity  $U$ , i.e.,  $D_L \propto U$ . However, *Dronfield and Silliman* [1993] reported that dispersion coefficient is proportional to velocity raised to the power  $n$ , i.e.,  $D_L \propto U^n$ , where  $n$  is 2 for parallel-plate fracture and 1.3 for rough fracture. *Roux et al.* [1998] also insisted that dispersion in rough fractures be described as the sum of three dispersion mechanisms: molecular diffusion, macrodispersion, and Taylor dispersion. Taylor dispersion is the main mechanism of solute dispersion caused by the parabolic velocity profile between the parallel-plate model, and Taylor dispersion coefficient is proportional to  $U^2$ . Macrodispersion occurs by variable aperture (i.e., fracture roughness) and is proportional to  $U$ . *Detwiler et al.* [2000] investigated the dependence of dispersion coefficient on Peclet number ( $Pe$ ) using experimental and numerical approaches, and confirms the conclusions of *Roux et al.* [1998]. *Detwiler et al.* showed that the relationship between dispersion coefficient and

$Pe$  is fitted by a quadratic equation, which combines macrodispersion (proportional to  $Pe^2$ ) and Taylor dispersion (proportional to  $Pe$ ):

$$\frac{D_L}{D_m} = \alpha_{Taylor} Pe^2 + \alpha_{macro} Pe + 1 \quad (1)$$

where  $D_m$  is molecular diffusion coefficient,  $\alpha_{Taylor}$  and  $\alpha_{macro}$  are nondimensional coefficients for the contributions of Taylor dispersion and macrodispersion, and  $Pe$  is

$$Pe = U \cdot b_m / D_m \quad (2)$$

where  $U$  is average flow velocity,  $b_m$  is mean aperture.

An induced-hydraulic gradient much higher than natural gradient is often necessary to clean up the contaminated groundwater, where non-Darcian flow is expected to occur. Under these circumstances, solute dispersion needs to be evaluated thoroughly for the full range of flow domains from Darcian to non-Darcian flows. In addition, a single solute was considered in deriving the relationship between  $D_L/D_m$  and  $Pe$ , although in field multi-solutes with different molecular diffusion coefficients often transport together through rock fractures. The purpose of this study is to examine the applicability of the  $D_L/D_m$ - $Pe$  relationship derived from a one-solute system to multi-solute situations under a full range of flow regime from Darcian to non-Darcian.

## 2. Methodology

The physics of fluid flow in fractures are often governed by the Navier-Stokes equations. These non-linear partial differential equations are difficult to solve. It is known that lattice Boltzmann method yields a close approximation to the Navier-Stokes equations [Chopard and Droz, 1998]. Therefore, this method was used to simulate solute transport in non-Darcian flow regime.

Natural rock fractures were used to simulate solute transport. Solute is instantaneously injected into the left end of the fracture and its concentration is monitored at the right end. We used two solutes in our numerical simulation. *Solute 2* has molecular diffusion coefficient two times higher than *Solute 1*:  $D_{m,Solute2} = 0.01 \text{ lu}^2/\text{ts}$  and  $D_{m,Solute1} = 0.005 \text{ lu}^2/\text{ts}$ , where  $lu$  and  $ts$  are lattice unit and time step. Hence, to have the same  $Pe$  for both solutes, the fluid velocity of *Solute 2* should be twice that of *Solute 1*. This implies that for the same  $Pe$ , the two solutes could be in different flow regimes; for example, *Solute 1* is still within Darcian flow domain but *Solute 2* could be in non-Darcian flow regime, which could lead to different  $D_L/D_m$  even at the same  $Pe$ .

The first and second moments,  $M_1$  and  $M_2$ , are the mean and variance of solute mass [Aris, 1956], and the rate of change of the second moment with time is twice the longitudinal dispersion coefficient.

## 3. Results

Fluid flow and solute transport simulations were conducted at various flow velocities (Figure 1). Velocity profile and the distribution of solute mass at the Reynolds number ( $Re$ ) of 30 are shown in Figures 1a and 1b, respectively. Darker regions

represent higher velocities (Figure 1a) or higher concentrations (Figure 1b), lighter corresponds to lower velocities or lower concentrations, and solid black near the fracture wall denotes zones with eddies. Fracture has local asperities, which contributes to forming eddies (Figure 1a). Eddies are observed from  $Re$  of 15. Lower velocity zones and turbulent flows are developed near the fracture wall (Figure 1a), which delay solute transport along the wall (Figure 1b). Figure 2a shows flow velocity versus particle acceleration. The product of acceleration and particle density per site specified in the simulation equals pressure gradient. The flow becomes non-Darcian from  $Re$  of 10 (Figure 2a), which corresponds to  $Pe$  of 100 for *Solute 2* and  $Pe$  of 200 for *Solute 1*. With increasing fluid velocity, the relationship between fluid velocity and applied acceleration deviates much larger from the linearity, mainly due to turbulent flow, which leads to a higher dispersion coefficient.

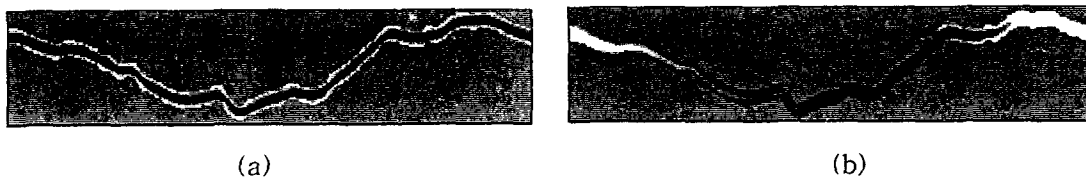


Figure 1. Fluid flow (a) and solute transport (b) simulations at  $Re$  of 30.

We examine the consequent solute transport in fractures. Figure 2b shows the relationship between  $D_l/D_m$  and  $Pe$ . We dropped 1 from equation (1) to fit the non-linear relationship between  $D_l/D_m$  and  $Pe$ . The 1 in equation (1) is related to molecular diffusion term which can be ignored at high  $Pe$ . It is found that  $D_l/D_m$ - $Pe$  relationship is well fitted by a quadratic equation for the flow domain including non-Darcian flow (Figure 2b), which means that Taylor and macro-dispersions are the main dispersion mechanisms in rock fractures for both Darcian and non-Darcian flow regimes.

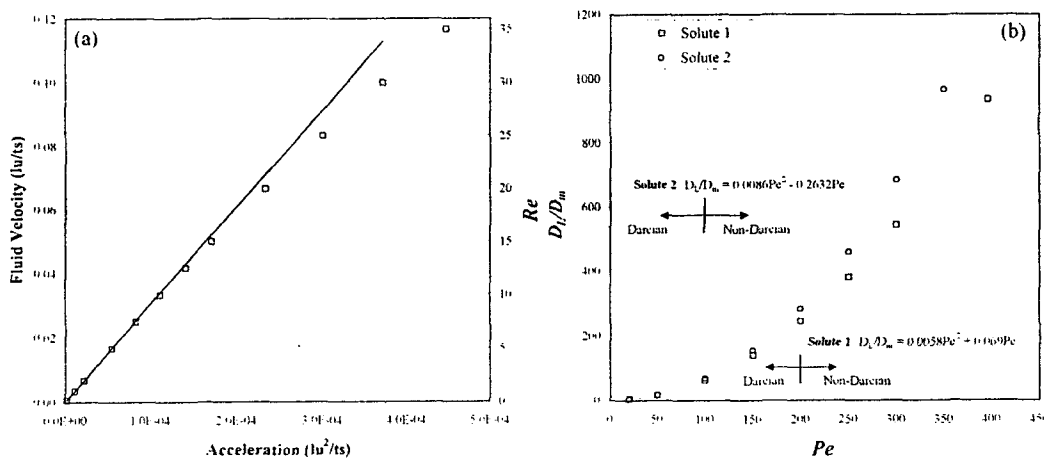


Figure 2. Fluid velocity versus applied acceleration (a) and  $D_l/D_m$  versus  $Pe$  (b).

*Solute 1* and *Solute 2* lead to the same  $D_l/D_m$  for  $Pe$  less than 100, which

is Darcian flow regime for both solutes (Figure 2b). But, as non-Darcian flow starts from  $Re$  of 10 corresponding to  $Pe$  of 100 for *Solute 2*, *Solute 2* yields different  $D_l/D_m$  at  $Pe$  higher than 100 from that of *Solute 1* (Figure 2b). The difference in  $D_l/D_m$  becomes large as non-Darcian flow increases by turbulent flow.  $\alpha_{Taylor}$  of *Solute 2* is higher than that of *Solute 1*, as turbulent flow becomes larger at *Solute 2* than at *Solute 1*.  $\alpha_{macro}$  of *Solute 2* is less than zero (Figure 2b). The formation of turbulent flow interferes with and delays solute transport along the fracture wall, which contributes to dropping  $\alpha_{macro}$  below zero.

#### 4. Conclusions

Most experimental studies of solute transport in rock fractures have been limited to Darcian flow regime with one solute. We examined a two-solute transport system under both Darcian and non-Darcian flow condition. We found that solute dispersion in rock fractures can be characterized by the mechanism of both macrodispersion and Taylor dispersion, even for non-Darcian flow domain. It is found that within Darcian flow regime, solutes with different molecular diffusion coefficients lead to the same  $D_l/D_m$  at same  $Pe$ . However, as the flow becomes non-Darcian, solute with a higher molecular diffusion coefficient leads to higher  $D_l/D_m$  than solute with a lower diffusion coefficient. Non-Darcian flow is composed of non-linear laminar and turbulent flows. Even for non-linear laminar flow without any turbulent flow, different solutes lead to the different relationship between  $D_l/D_m$  and  $Pe$ . When non-Darcian prevails in rock fractures, it leads to the increase of  $\alpha_{Taylor}$  and the decrease of  $\alpha_{macro}$ . Since in fact, numerous solutes exist and disperse together in rock fractures, this study suggests that it is necessary to thoroughly evaluate the transport behavior of individual solute in rock fractures, especially when the flow is non-Darcian.

#### References

- Aris, R., On dispersion of a solute in a fluid flowing through a tube, *Proc. R. Soc. London A*, 235, 66-77, 1956.
- Chopard, B. and M. Droz, *Cellular automata modeling of physical systems*, 341 pp., Cambridge University Press, New York, 1998.
- Detwiler, R. L., H. Rajaram, and R. J. Glass, Solute transport in variable-aperture fractures: an investigation of the relative importance of Taylor dispersion and macrodispersion, *Water Resour. Res.*, 36(7), 1611-1625, 2000.
- Dronfield, D. G. and S. E. Silliman, Velocity dependence of dispersion for transport through a single fracture of variable roughness, *Water Resour. Res.*, 29(10), 3477-3483, 1993.
- Keller, A. A., P. V. Roberts, and M. J. Martin, Effect of fracture aperture variations on the dispersion of solutes, *Water Resour. Res.*, 35(1), 55-63, 1999.
- Roux, S., F. Plouraboue, and J. P. Hulin, Tracer dispersion in rough open cracks, *Trans. Porous Media*, 32, 97-116, 1998.