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Research paper

Experimental study and characteristic finite element simulation of solute transport in a cross-fracture

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Long-fei Chen [a], Yong Huang [b,*]

[a] Civil Engineering Department of Chongqing Three Gorges College, Wanzhou 404000, China
[b] School of Earth Sciences and Engineering, Hohai University, Nanjing 210098, China

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ABSTRACT

A new method, the characteristic finite element method (CFEM), was developed to simulate solute transport in a cross-fracture. The solution of this mathematical model for solute transport considered that the contribution of convection and dispersion terms was deduced using the single-step, trace-back method and routine finite element method (FEM). Also, experimental models were designed to verify the reliability and validity of the CFEM. Results showed that experimental data from a single fracture model agreed with numerical simulations obtained from the use of the CFEM. However, routine FEM caused numerical oscillation and dispersion during the calculation of solute concentration. Furthermore, in this cross-fracture model, CFEM simulation results predicted that the arrival time of concentration peak values decreased with increasing flux. Also, the second concentration peak value was obvious with the decrease of flux, which may have resulted from the convergence of solute concentrations from main, and branch, fractures.

1. Introduction

Simulation methods of solute transport in cross-fractures include analytical and numerical schemes. For example, Park and Kang (1999) provided an analytical solution for solute transport in 2-D perpendicular fractures; however, their method can only be applied to simple boundary conditions. In fact, fracture distribution and geometric characteristics are considerably more complex compared to fractured rocks matrices. It is difficult to deduce an analytical solution to the problem of solute transport in cross-fracture or in a fracture network. Therefore, a numerical scheme is usually employed to simulate the behaviour of cross-fractures. Zhang et al. (2008) used FEM to solve the Navier-Stokes equation in a cross-fracture. Also, a complex pipe network model was used to simulate its hydraulic and migration properties.

Except for these routine numerical methods, some new, or modified, schemes were proposed to solve mathematical models of solute transport. For example, Guo et al. (2009) proposed a new characteristic-based finite volume scheme which combined reconstruction and the characteristics of a central weighted essentially non-oscillatory flow so as to simulate dam-break problems. Fracture boundary extraction was developed by Tan and Zhou (2008) and Tan et al. (2009) using a Gaussian template and canny boundary detection based on collected digital images of natural fractures. An Eulerian-Lagrangian approach, with particle tracking for groundwater flow analysis, was used to handle vertical flow under variably saturated conditions (Gennady et al., 1998; Zhang et al., 2008); however, it did not consider solute transport. Also, the rough fracture surface and the distribution of fracture apertures were simulated by Wang and Zhou (2004) based on fractal theory. Seol et al. (2003) investigated fracture-matrix systems for a 2-D parallel plate and considered the influence of different degrees of saturation on the solute transport therein. Fracture-matrix interactions were simulated by Yu et al. (2004) using a physical approach. Furthermore, stochastic schemes have been applied to the simulation of solute transport in fractures (Bodin et al., 2007; He et al., 2007).

To avoid numerical oscillation and dispersion using routine FEM during the calculation of solute concentrations, a CFEM scheme has been developed to simulate contaminant migration in fractures. Also, experiments were established to verify the validity and

* Corresponding author.
E-mail address: hyong@hhu.edu.cn (Y. Huang).
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reliability of the method. Furthermore, the sensitivity of flux through the fractures to solute concentration was analysed to assess the influence of a branch fracture on the main fracture.

2. CFEM schemes

This CFEM was developed on the basis of the FEM. It can simulate groundwater in fractured rocks using a continuum medium model (Zhou, 2003) and has been applied and verified in many major hydropower engineering projects in China, such as the Xiluodu hydropower station, the Three Gorges dam project, at Longtan hydropower station, and on the Huizhou pumped-storage power station (Huang et al., 2013).

The control equation of solute transport in the fractured medium can be described by

$$R_d\frac{\partial C}{\partial t} = \nabla\cdot(D\cdot\nabla C - uC) - \lambda R_d C + W \tag{1}$$

where R_d is the retardation factor, C is the solute concentration, t is time, ∇ is the Hamiltonian differential operator, D is the hydrodynamic dispersion coefficient tensor, u is the velocity of groundwater flow, λ is the radioactivity decay constant, and W represents the sources and sinks of the solute mass.

The hydro-dynamical derivative, D/Dt, is defined as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{u\cdot\nabla}{R_d} \tag{2}$$

So, Eq. (1) can be

$$R_d\frac{DC}{Dt} = \nabla\cdot(D\cdot\nabla C) - fC + W \tag{3}$$

where,

$$f = \nabla\cdot u + \lambda R_d \tag{4}$$

It is noted that the concentration, C, in Eq. (3) does not represent the spatial concentration at a point, but instead denotes the concentration of solute with velocity u/R_d. Therefore, the solution of Eq. (1) is divided into two parts which consisted of the contributions from its convection and dispersion terms. For simplicity, the 2-D solution will be deduced to demonstrate how to solve Eq. (3) using the CFEM.

2.1. Characteristic solution of convection term

Eq. (2) can be solved using the characteristic curve method; the characteristic equation is expressed by Eq. (5):

$$\frac{dX}{dt} = \frac{u}{R_d} = u_k \tag{5}$$

If each node were considered to be a kinetic particle, and the direction of movement thereof was in opposition of that of the groundwater flow, it may be assumed that there exists an imaginary particle for each node. Such a particle will move to point $P(x_i, y_i)$ under the action of convection after time, Δt. The situation is expressed by Eq. (6):

$$\begin{cases} x_i^k = x_i^{k+1} - \int_k^{k+1} u_x^k dt \\ y_i^k = y_i^{k+1} - \int_k^{k+1} u_y^k dt \end{cases} \tag{6}$$

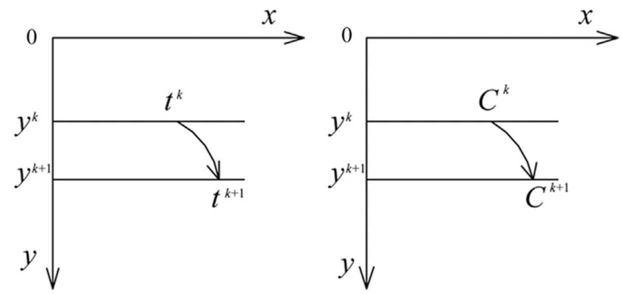

Figure 1. Sketch map of the single step trace-back method.

where x_i^{k+1} and y_i^{k+1} are the coordinates of particle i at t^{k+1}, u_x^k and u_y^k represent the velocity component of particle i along the x- and y-directions, respectively. So, the location of particle i at t^k can be tracked using the location of particle i at t^{k+1}, which is called the single step trace-back method (Fig. 1). The second term on the right-hand side of Eq. (6) is calculated by mean value theorem, therefore:

$$\begin{cases} x_i^k = x_i^{k+1} - \dfrac{u_x^k\left(x_i^k, y_i^{k+1}, t^k\right) + u_x^k\left(x_i^k, y_i^{k+1} - \Delta t u_x^k, t^k\right)}{2}\cdot\Delta t \\ y_i^k = y_i^{k+1} - \dfrac{u_y^k\left(x_i^k, y_i^{k+1}, t^k\right) + u_y^k\left(x_i^{k+1} - \Delta t u_y^k, y_i^k, t^k\right)}{2}\cdot\Delta t \end{cases} \tag{7}$$

If the location of particle i at t^k has been determined by Eq. (7), the contribution of convection term, $\overline{C_i^k}$, can be calculated by interpolation across each element, that is

$$\overline{C_i^k} \approx \sum_{i=1}^{NN} \varphi_i\left(x_i^k, y_i^k\right) C_i^{k-1} \tag{8}$$

where NN is the number of nodes for an element, φ is the basic function.

2.2. Solution of dispersion term by FEM

According to the Galerkin method, Eq. (3) may be expressed as

$$\iint_\Omega \left[R_d\frac{DC}{Dt} - \nabla\cdot(D\cdot\nabla C) + fC - W\right]\varphi_i dxdy = 0 \quad (i = 1, 2, \cdots, NP) \tag{9}$$

where, Ω is a domain, and NP is the total number of nodes. Based on the FEM, the approximation solution for concentration, $\widetilde{C}$, is given by

$$\widetilde{C} \approx \sum_{i=1}^{NN} \varphi_i C_i \tag{10}$$

Substituting Eq. (10) into Eq. (9), Eq. (9) could be rewritten as

$$\iint_\Omega \left[R_d\frac{D\widetilde{C}}{Dt} - \nabla\cdot\left(D\cdot\nabla\widetilde{C}\right) + f\widetilde{C} - W\right]\varphi_i dxdy = 0 \quad (i = 1, 2, \cdots, NP) \tag{11}$$

The two ranks partial derivative of Eq. (11) can be solved using Green's formula, and $D\widetilde{C}/Dt$ can be approximated by the difference, that is