Characterizing Non-Fickian Transport in Fractured Rock Masses Using Fractional Derivative-Based Mathematical Model

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Keywords

Mass transport, tracer test, fracture network, fractional derivative, non-Fickian diffusion, fractal geometry

ABSTRACT

A fractional advection-dispersion equation (fADE) was employed to describe non-Fickian mass transport in fractured rock masses. A fracture network model based on fractal geometry was utilized to analyze numerical tracer responses in inhomogeneous rock masses composed of a number of natural fractures. The density of the natural fractures was varied in the numerical analyses. It was shown that non-Fickian transport (anomalous dispersion with heavy tails) was observed for lower natural fracture densities and the tracer response could be described by the fADE. It was suggested that the term of fractional time derivative in the fADE was responsible for the variance of travel time in the tracer responses, resulting in the non-Fickian transport. The results obtained in this study may support the use of the fADE for characterizing complex fluid flow in geothermal reservoirs.

Introduction

Reinjection started originally as a disposal method in the development of conventional geothermal resources. However, it has more recently been recognized as an essential and important part of reservoir management and has been included in enhanced geothermal systems (EGS). Computer models (e.g., TOUGH2 (Pruess, 1991)) are often employed for reservoir analyses, which require the details of structural description, stratigraphy, reservoir parameters, etc. However, it is usually time-consuming and costly to obtain sufficient field data for such analyses in most geothermal sites.

In this study, we are interested in tracer tests which help monitor fluid movement within the reservoir. Tracers play an important role in the exploration and characterization of geothermal resources, and can also be a valuable tool in the design and management of production and injection operations. Tracer tests are expected to provide useful and convenient information for characterizing globally the underground structure through the mass transport between injection and production wells, whilst the other many methods can collect data only in the vicinity of exploration wells.

The advection–dispersion equation (ADE) commonly used to describe mass transport in aquifers is given as follows:

$$\frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} \tag{1}$$

where c is the solute concentration, v the average linear velocity, x the distance, τ the time, and D the diffusion coefficient, respectively. However, the ADE generally underestimates concentrations in the leading and/or trailing edges of tracer responses both in the laboratory and in the field (Hatano et al., 1998; Berkowitz et al., 2000; A. Cortis and B. Berkowitz, 2004). Dispersion of tracers in natural systems is typically observed to be anomalous diffusion that is not always appropriately described by Fick's law. The transport is called "non-Fickian". Numerous authors have shown the equivalence between the non-Fickian motions and transport equations that use fractional-order derivatives (Benson et al., 2000; Zhang et al., 2009; Fomin et al, 2010). We focus on the fractional advection-dispersion equation (fADE), which predicts the mass transport in fractured reservoirs. A schematic sketch of fractured porous aquifer envisioned in this study is presented in Figure 1, together with the fADE. The equation, which is already dimensionless and normalized, is written as follows (Chiba et al., 2008):

$$\frac{\partial C}{\partial T} + b\frac{\partial^\gamma C}{\partial T^\gamma} + \frac{\partial^\beta C}{\partial T^\beta} = \frac{1}{Pe}\frac{\partial}{\partial X}\left(\frac{\partial^{\alpha-1} C}{\partial X^{\alpha-1}}\right) - \frac{\partial C}{\partial X} \tag{2}$$

where C is the concentration in the liquid, X the transverse spatial coordinate, T the time, b the capacity coefficient for the fractional derivative, Pe the Peclet number, α, β, γ fractional time and space derivatives ($1.0 < \alpha \leqq 2.0$, $0.0 < \beta < 0.5$, $0.0 < \gamma \leqq 1.0$), respectively. The second term on the left-hand side of Equation (2) models the retardation process associated with secondary branched fractures and matrix permeability. The third term on the left-hand side is the process of vertical dispersion into surrounding

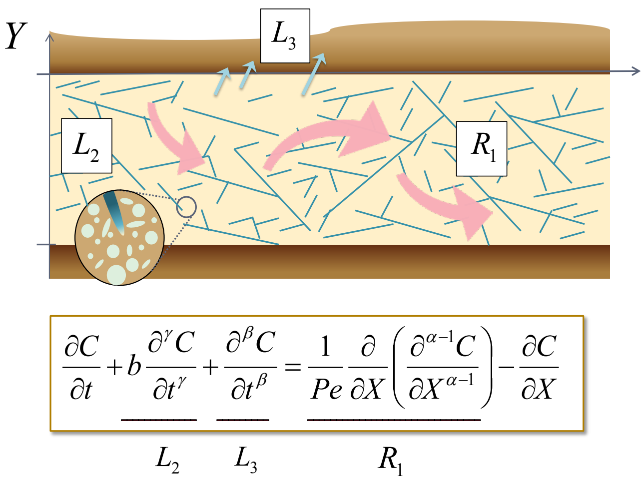

Figure 1. Schematic of the fADE in a fractured porous aquifer.

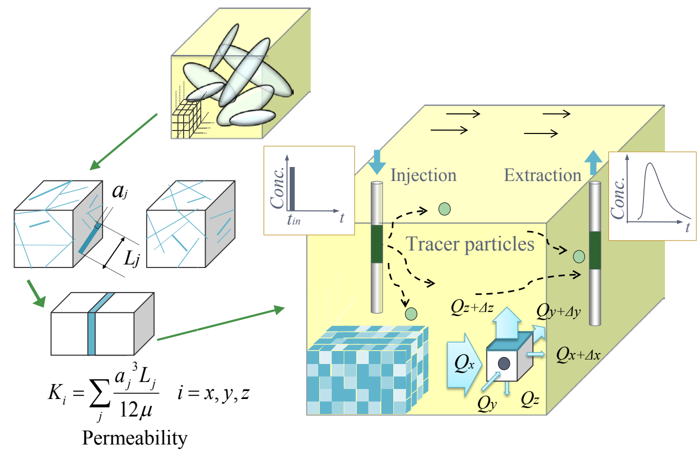

Figure 2. Schematic of tracer response analysis based on the fractured reservoir model.

rock masses. The first term on the right-hand side expresses the dissipation in the direction water flow.

The fractional derivative terms with respect to time and space describe the nonlocal dependence on time and space. Here, the concentration change at some location and time might depend on a wide variety of locations in space (i.e., the space nonlocality), and also might depend on the temporal history of concentration "loading" at that location (the time nonlocality). The time nonlocality can explain mass decline because it describes the dynamic partitioning of solute mass into the immobile phase, while the space nonlocality cannot distinguish the status of solutes (Zhang et al, 2009). The nonlocalities can express the development of anomalous dispersion. As yet, little work has been done on the relashinship between the nonlocalities and the stuructures of fractured rock masses.

We utilize a mathematical model (fADE) to develop a "comprehensive and panoramic" model for describing mass transport in fractured rock masses in this study. The constitutive variables in the fADE are determined for mass transport obtained using a fracture network model based on fractal geometry. The effects of fracture densities on the constitutive variables are then discussed.

Numerical Analysis

Analysis Method of fADE

The finite-difference method (FDM) is a well-known numerical method that has been applied to the ADE (Meerschaert and Tadjeran, 2004). We performed the numerical solution of Equation (2) by implicit FDM. In this work, the fractional derivative in the governing differential equation is formulated with Caputo's fractional derivative (Caputo, 1967; Zhang et al., 2007).

Fracture Reservoir Model

A 3D stochastic fracture network model based on fractal geometry is employed to analyze numerical mass transport in inhomogeneous fractured rock masses and further developed to perform tracer analyses in this study. The schematic of fracture network model and tracer response analyses is illustrated in Figure 2 (Jing et al., 2000).

In order to perform analyses of tracer tests, a distribution of fractures with a circular shape is constructed in a 3D calculation region, first. The fracture radius, r_η, is generated based on the fractal geometry using the following equation:

$$r_\eta=\left[(1-\eta)r_{\min}^{-D}+\eta r_{\max}^{-D}\right]^{-1/D} \tag{3}$$

where η is a random number in the range 0.0 to 1.0, D the fractal dimension that has been proven to be capable of mathematically representing the geometry of natural fractures (Watanabe and Takahashi, 1995), r_{min} and r_{max} the specified radius of the smallest and largest fractures in the model, respectively. Fractures are generated until the fracture density reaches the determined level. The number of fractures, N, is then given by:

$$N=C\left[r_{\min}^{-D}-r_{\max}^{-D}\right] \tag{4}$$

where C is the fracture density parameter. The locations and orientations of individual fractures are assumed to be random. Furthermore, it is assumed that the aperture of circular fracture, a_i, is proportional to its radius.

In the 3D model, the flow analyses are conducted on a square grid and the network model is solved by converting the network to an equivalent continuum mesh, as illustrated in Figure 2. To model fluid flow within a natural reservoir, we set up calculations in the x, y, and z directions in a 100m×100m×70m domain on a 100×100×70 grid. The Distribution of permeability for each block surface, K_i, is governed by the sum of product from each penetrating fractures, as follow:

$$K_i=\sum_{j=1}^{N}\frac{a_j L_j}{12\mu}, \quad i=x,y,z \tag{5}$$

where a_i is the fracture aperture, L_i the fracture intersection length, and η is viscosity of water. Fluid flow is assumed to be laminar and controlled by Darcy's law and the continuity equation:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial P}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial P}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial P}{\partial z}\right)=0 \tag{6}$$

Flow calculations are carried out based on Equation (6) under the boundary conditions as depicted in Figure 3. A natural fluid flow is assumed to take place from the injection point toward the production point, and the pressure along the edge for the inlet

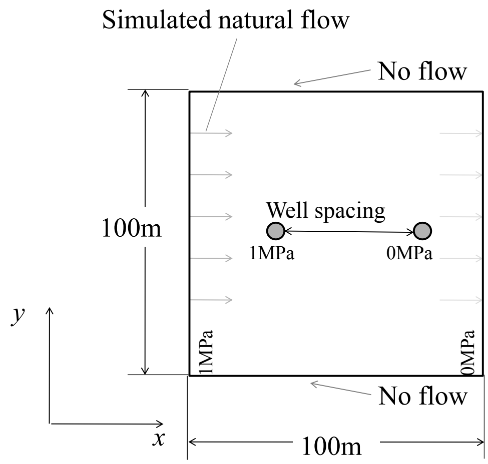

Figure 3. Calculation conditions of the fractured reservoir model.

side is taken as 1MPa and that for the outlet side 0MPa. No-flow conditions are assumed at the other edges. The pressure at the inlet well is set to be 1MPa and that for the outlet well 0MPa.

The tracer analyses are based on the premise that tracer substances are particle ensembles and each tracer particle travels from the injection well to the extraction well located in the above flow. Now, a particle continues to move in the direction decided by probability approach with respect to volume flow rate. Frequency distribution of tracer particles is expressed as the rate of extraction particles sorted by the travel time to total particles. The relative concentrations of tracers are then calculated as the ratio of particle flux during one time interval to total particle flux:

$$C(x,t) = \frac{N_p / Q_p \Delta t_p}{N_{all} / Q_{in} t_{in}} \tag{7}$$

where N_p is the number of extracted particles during one time interval, Q_p the extraction flow rate, Q_{in} the injection flow rate, Δt_p the time interval, and t_{in} the injection time, respectively. In this analysis, the fracture densities are varied in order to fractured reservoirs different complexities. The parameters used for the simulations are listed in Table 1.

Estimation of fADE Constitutive Parameters

The fADE is then used to characterize the tracer responses obtained by conducing the flow analyzes in the fractured reservoir. The characterization requires the determination of the constitutive parameters in the fADE such as α, β, γ, b and Pe. In order to determine the fADE constitutive parameters, an optimization proceedure was executed using Automatic Design Synthesis (ADS) (Vanderplaats and Sugimoto, 1986). Note that the third term of the left hand side in Equation (2) describes the dissipation from the aquifer to the surrounding rocks. In this study, however, no optimal solution was obtained with the third term, which may suggest the dispersion into the calculation region outside the injection interval was negligible. Thus, only α, γ, b and Pe in the fADE were optimized. It has been shown that no optimal solution was obtained with the ADS for four unknown parameters. Hence, an initial value for α was selected first and the other three constitutive parameters were optimized by the ADS for the assumed value of α. The solution for α was found by changing systematically the value of α and repeating the above-mentioned optimization with the ADS (see Figure 4).

Table 1. Parameters used for the simulation.

Parameters		Value
Fractal dimension		1
Fracture radius	r [m]	0.5～25
Fracture aperture	[m]	$1.0\times10^{-4}\times r$
Well spacing	[m]	50
Well length	[m]	50
Injection pressure	[MPa]	1
Production pressure	[MPa]	0
Matrix permeability	[m^2]	1.0×10^{-14}
Viscosity of water	[Pa·s]	10^{-2}
Number of tracer particles		1.0×10^4

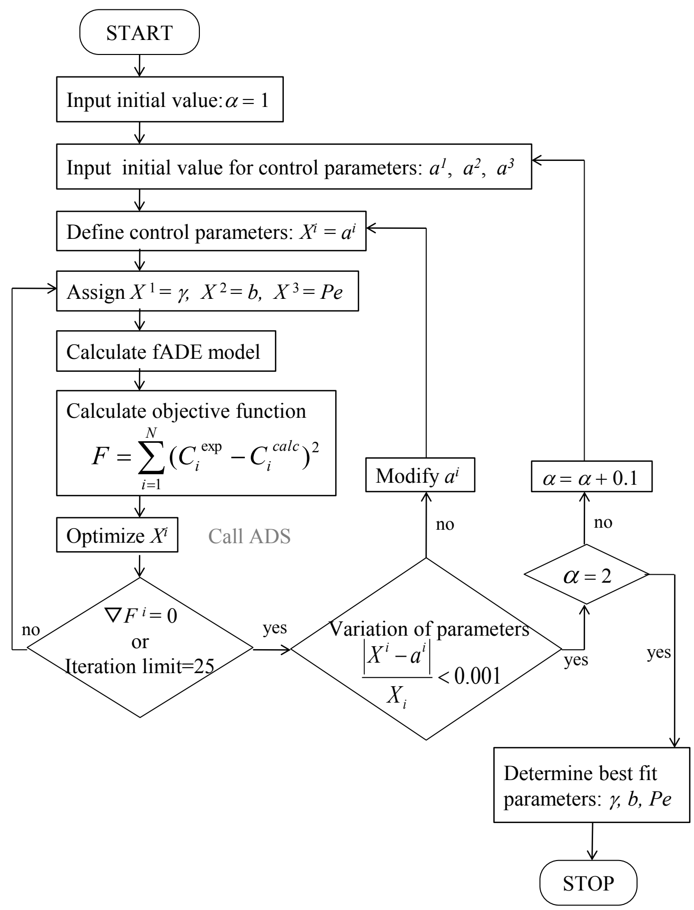

Figure 4. Calculation flow of the optimization procedure using ADS.

The optimization with the ADS is based on the Davidon-Fletcher-Powell (DFP) variable metric method for unconstrained minimization and finds the minimum of an unconstrained function using the Golden Section method. Initial values a^i (i=1, 2, 3) for the fADE constitutive parameters to be optimized are assumed and given first. The given parameters are assigned to the control parameters X^i (i=1, 2, 3) to carry out the optimization. The fADE is solved and its solution is then compared with the numerical result obtained by the fractured reservoir analysis. An objective function, F, is defined as follows:

$$F = \sum_{i=1}^{N} \left(C_i^{\exp} - C_i^{calc} \right)^2 \tag{8}$$

where $C_i^{\exp}$ is the numerical data of concentrations obtained from the tracer analyses using the fractured reservoir model, C_i^{calc} the numerical solution of the fADE, and N the number of data points for concentration, respectively. The ADS is then employed in order to implement the optimization by using finite difference gradients ∇F^i. If $\nabla F^i = 0$ or the number of iterations exceed 25, the variations of the updated control parameters X^i with respect to the initial control parameters a^i are then evaluated and the calculation step is repeated for the updated a^i until the relative variation of the parameters meet the requirement, as indicated in Figure 4. The above-mentioned process is iterated in order to find the optimal value for α which gives the minimum objective function.

Results and Discussion

The distribution of travel times computed from the tracer analyses was examined first. The frequency distributions are expressed in terms of the probability density. When the fracture density exceeds 20,000, the peak in the distributions appears at the travel time of around 10^3s. In the case of the fracture density range, it was observed that the tracer particles always traveled through the fracture network. In contrast, when the fracture density is lower than 20,000, the other peak appears after 10^6s. The second peak is attributable to the matrix permeability assigned for the whole calculation area. When the fracture density becomes much lower (C < 1,000), only the second peak due to the matrix permeability remains, eliminating the first peak. In view of the travel time distributions, the results for the fracture densities (C = 5,000 ~ 50,000) in which the first peak appears will be discussed below.

The advection-dispersion equation (ADE) with $\alpha = 2.0$, $\gamma = 1.0$ was applied to fit the tracer break through curves using the above-mentioned optimization method. The curve fitting allows us to look at the applicability of Fick's law. Correlation coefficients, R^2, between the results of the tracer breakthrough curves and the numerical solutions are given by:

$$R^2 = 1 - \frac{\sum_{i=1}^{N} \left(C_i^{\exp} - C_i^{calc} \right)^2}{\sum_{i=1}^{N} \left(C_i^{\exp} - C_{ave} \right)^2} \tag{9}$$

where C_{ave} is the average concentration for the prescribed travel time. The correlation coefficient is plotted against the fracture density in Figure 6. The correlation coefficients show a value close to 1.0 when the fracture density is greater than 20,000. Thus, the tracer behavior can be regarded as Fickian for the higher fracture density range. The reason for this may be caused by the fracture distribution in the rock masses tends to become more or less uniform and ubiquitous with a number of fractures. On the other hand, when the fracture density decreases, the correlation coefficient reduces rapidly and becomes almost zero at the lowest fracture density. In the case of the lower fracture densities, the tracer behavior can be regarded as non-Fickian, and no reasonable description can be provided by Fick's law. The inhomogeneous distribution of fractures with the low fracture densities is considered to cause the non-Fickian behavior.

The fADE was used to fit the break through curves, using the optimization method. The fitted curves are shown in Figure 7, for the selected fracture densities. The travel time was normalized with the averaged value of the tracer travel times, which was

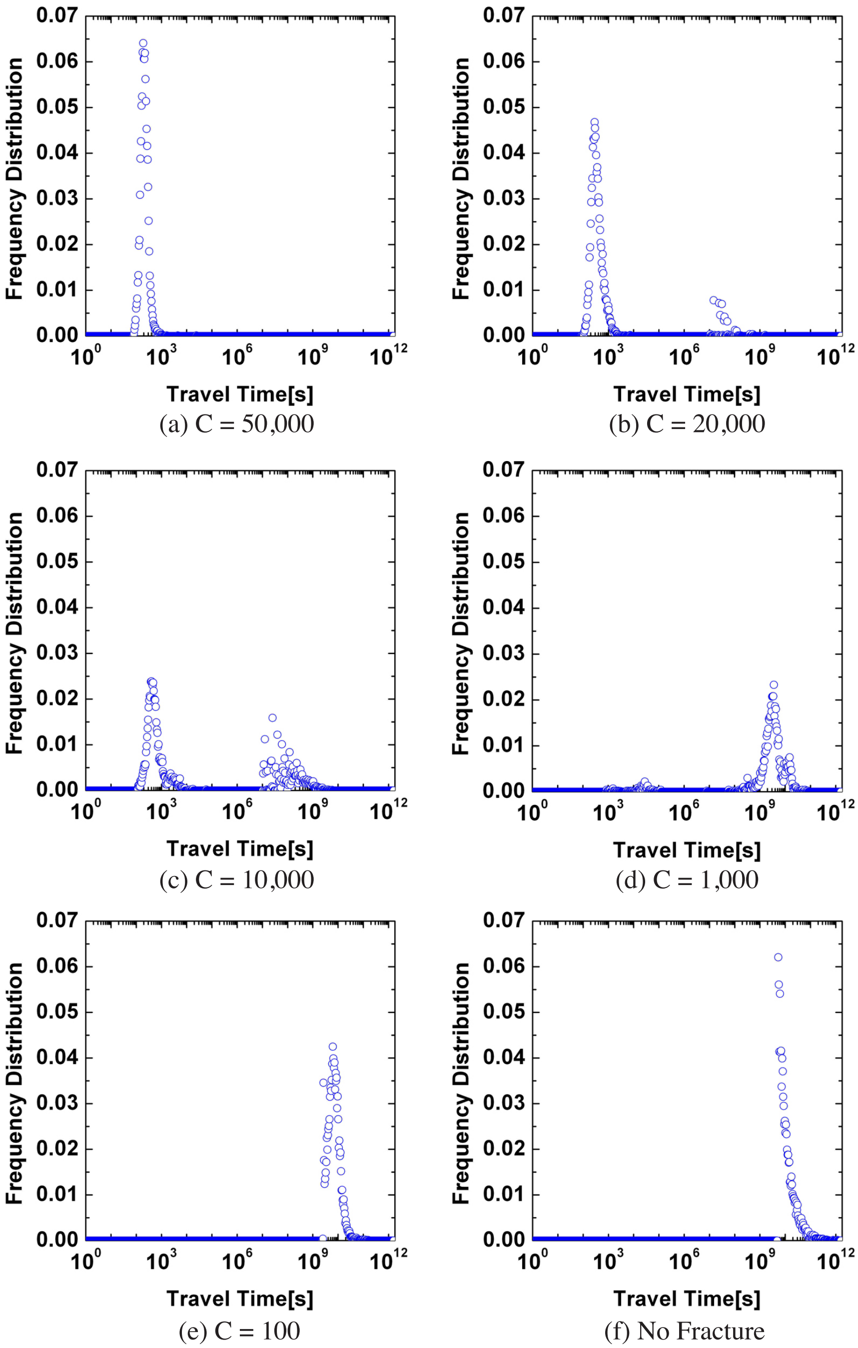

Figure 5. Frequency distribution versus travel time for fracture distribution with different fracture densities.

calculated using the first 20% of the total particles reached at the outlet. The results show that the solutions of the fADE provide a surprisingly good approximation to the tracer break through curves, even for the non-Fickian responses. As given in Figure 6, the correlation coefficient is close to 1.0 even for the lower fracture densities (C < 20,000). Thus, it is understood that the fADE provides a useful means for characterizing the tracer responses in the fractured rock masses.

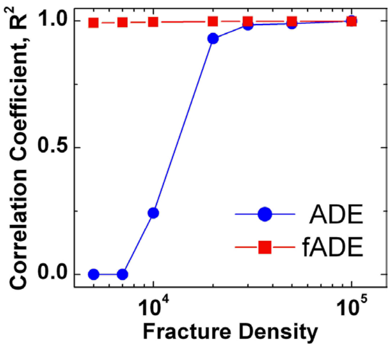

Figure 6. Applicability of the ADE to results of tracer responses with different fracture densities.

Figure 8 summarizes the best-fit constitutive variables in the fADE, including the space scale index α , the time scale index γ, and the fractional capacity coefficient *b*, as a function of different fracture densities. The numerical result shows that the best-fit value of α, which is an order of the space derivative, exhibits a complicated trend of variation with the fracture density, with α being less than 2.0. Further investigation is underway in order to clarify the relationship between α and the structure of rock masses.

It is noted that γ is approximately equal to 1.0 for the higher fracture densities (C>20,000) and *b* gives an almost constant value, as shown in Figure 8. The integer value of γ indicates that the mass transport is Fickian, as discussed in Figure 6. When the fracture density becomes less than 20,000, γ reduces and *b* increases for the decreasing fracture density. The value of non-integer for γ indicates that the mass transport becomes non-Fickian with the lower fracture densities. When the fracture density decreases, the variance of the tracer travel time increases as shown in Figure 9. A good approximation by the fADE demonstrates that the nonlocalities described by the time fractional derivative in the fADE can offer an appropriate mathematical description for the temporal fluctuation of tracer responses and the temporal heterogeneity.

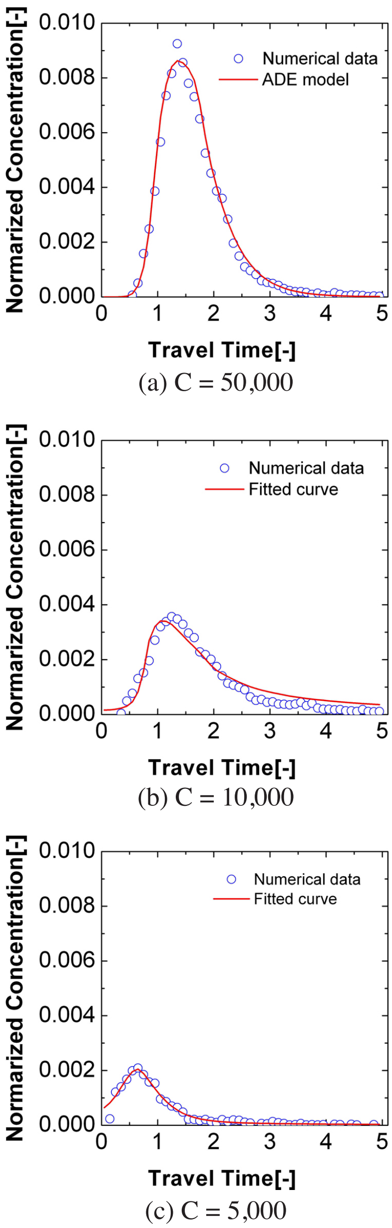

Figure 7. Comparison between numerical result from the fracture reservoir model (open symbols) and analytical solution by the fADE (solid line).

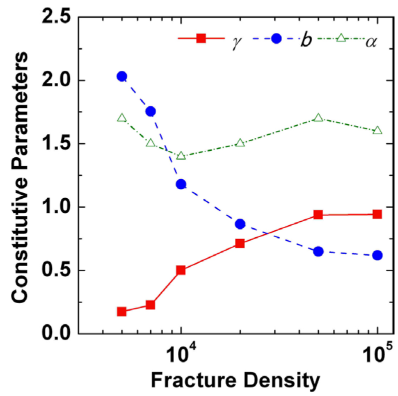

Figure 8. Fracture density versus best-fit variables in the fADE (including α, γ and b).

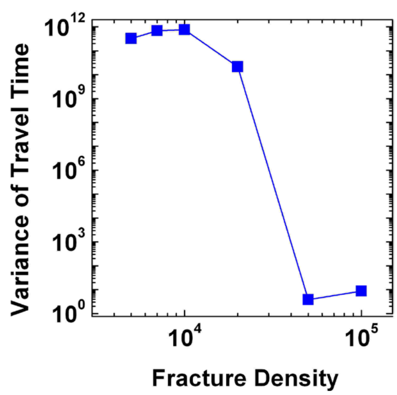

Figure 9. Fracture density versus variance of tracer travel time.

Concluding Remarks

The fractured reservoir 3D model with fracture networks has been designed and developed to facilitate analyzing tracer tests. The techniques developed here can also be used to study the mass transport in natural reservoirs through fractal geometry and matrix permeability.

Our simulations of tracer tests in fractured reservoirs produce not only Fickian but also non-Fickian transport, which is generally shown in field observations. The shift of transport behaviors depend on fracture density. The fractional advection-dispersion equation provides a simple and accurate predictive model for tracer behavior in fractured reservoirs that exhibit heterogeneity. The non-Fickian transport will influence the temporal fluctuation caused by nonlocalities.

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