Numerical Simulations of the Anomalous Solute Transport in a Fractured Porous Aquifer

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Anomalous contaminant transport, non-Fickian diffusion, fractional derivative, fractured porous media

ABSTRACT

A computer program, which enables us to calculate the anomalous non-Fickian contaminant transport in complex medium, has been developed. In recent years, prediction of mass transport in fractured porous media is becoming increasingly more important for the development of subsurface energy and material systems such as geothermal energy system and the geological disposal of radioactive wastes. Solute transport simulation can serve as an effective tool for predicting subsurface fluid flow but requires accurate model derivation and reliable values of physical parameters. The conventional mathematical model of contaminant transport in the aquifer is based on the Fick's law of diffusion. However, for the fractured porous media, where solute moves primarily through open channels and slowly diffuses into the porous blocks, the conventional model tends to predict smaller solute travel distance than that in the actual transport process. In contrast, the non-Fickian diffusion model can provide realistic representation of actual fluid flow in the heterogeneous media, such as fractured porous rocks. In the non-Fickian diffusion model, the governing equation is written in terms of fractional derivatives. In this study, in order to expand the applicability of the non-Fickian diffusion model to a variety of practical engineering problems, a numerical method has been developed. We provide a numerical solution of the equations by using implicit-finite difference method. The results obtained by numerical solution of the fractional differential equations were shown to be in a good agreement with analytical solutions.

Introduction

A numerical method, which enables us to calculate the non-Fickian solute transport in a fractured porous aquifer, has been developed. In recent years, prediction of mass transport in fractured porous media is becoming increasingly more important for the development of subsurface energy and material systems such as the geothermal energy system and the geological disposal of radioactive wastes.

Unfortunately, as has been proven by a number of field and laboratory experiments, traditional constitutive equations (such as Fick's law) and corresponding mathematical models, which are based on second order partial differential equations, do not always work well for modeling mass transport in complex heterogeneous fractured rocks (Keller *et al*. 1995)) and, therefore, new reliable models and approaches are needed. In this study, we present the mathematical model for the anomalous mass transport in fractured porous aquifer, which is based on fractional order differential equations, and solve it numerically. We provide a numerical solution of the equations by using implicit-finite difference method.

Fractional Derivative

The non-Fickian contaminant transport model is described by using fractional derivative. In fractional derivative, differential coefficients are described as noninteger number. The theory of the fractional derivative was developed more than 200 years ago, and several definitions have been developed (Samko *et al*. (1993)). In this study, we adapted the Caputo fractional derivative (Caputo(1967));

$$ {}_{a}^{C}D_{x}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha - n)} \int_{a}^{x} \frac{f^{(n)}(\xi)}{(x-\xi)^{\alpha+1-n}} d\xi \tag{1} $$

where, $\Gamma(x)$ is the Gamma function, and α the differential coefficient. To differentiate a fractional derivative equation, we used binomial theorem. From binomial theorem, for example, the Riemann-Liouville fractional derivative is differentiated as follows;

$$ \frac{\partial^{\alpha} f}{\partial x^{\alpha}} \approx \frac{1}{(\Delta x)^{\alpha}} \sum_{i=0}^{j+1} \frac{\Gamma(-\alpha + i)}{\Gamma(-\alpha)\Gamma(i+1)} f_{j-(i-1)} \tag{2} $$

Similarly, the Caputo fractional derivative can also be differentiated taking the initial value into consideration(Chiba *et al*.(2006)).

Numerical Approximation

Governing Equation

In this study, to expand the applicability of the non-Fickian diffusion model to a variety of practical engineering problems, a numerical method has been developed on the basis of fractional advection-dispersion equations. We take advantage of the Caputo fractional derivative equation in order to develop the numerical method for analyzing the fractional advection-dispersion equation in the fractured porous media. We provide a numerical solution of the fractional advection-dispersion equation using implicit-finite difference method. All numerical codes are written on Fortran 90.

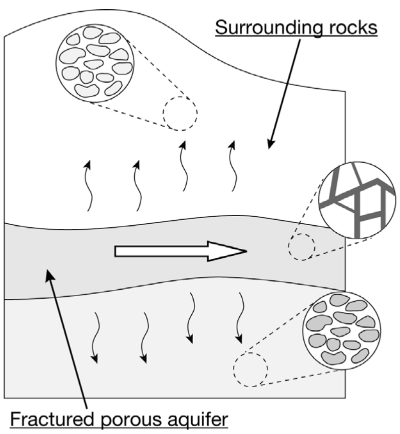

Figure 1. Schematic model of fractured porous aquifer.

Figure 1 is a conceptual model of fluid flow in the fractured porous aquifer. In the *x*-direction of Figure 1, we adapted the following fractional advection-dispersion equation to describe contaminant transport in the fractured porous aquifer by using the Caputo fractional derivative (Fomin *et al*.(2005));

$$\frac{\partial c}{\partial \tau}+\frac{\partial^{\gamma} c}{\partial \tau^{\gamma}}=-v\frac{\partial c}{\partial x}+D_1\frac{\partial}{\partial y}\left(\frac{\partial^{\alpha} c}{\partial y^{\alpha}}\right)+D\frac{\partial}{\partial x}\left(\frac{\partial^{\alpha} c}{\partial x^{\alpha}}\right) \tag{3}$$

On the other hand, anomalous mass transport in the surrounding rocks is described the following equation;

$$\frac{\partial^{\lambda} c_1}{\partial \tau^{\lambda}}=D_2\frac{\partial}{\partial y}\left(\frac{\partial^{\zeta} c_1}{\partial y^{\zeta}}\right) \tag{4}$$

where, c and c_1 are the concentration of solute in the fractured porous aquifer and the surrounding rocks, respectively; $D[\mathrm{L}^{1+\alpha}/\mathrm{T}^{-1}]$, $D_1[\mathrm{L}^{1+\alpha}/\mathrm{T}^{-1}]$ and $D_2[\mathrm{L}^{1+\zeta}/\mathrm{T}^{-1}]$ are effective diffusivities; $v[\mathrm{LT}^{-1}]$ is the fluid velocity; $\tau[\mathrm{T}]$ is time, and $0<\alpha, \gamma, \zeta, \lambda<1$. The order of fractional derivative α is close to 0, when the aquifer is a highly heterogeneous media. On the other hand, $\alpha = 1$ is assumed when the media becomes homogeneous. γ predicts the continuous transfer of contaminant from mobile to immobile phase -(Schumer *et al*.(2003)).

Numerical Approximation

Equation (3) and (4) were converted to the non-dimensional form;

$$\frac{\partial C}{\partial t}+b\frac{\partial^{\gamma} C}{\partial t^{\gamma}}+\frac{\partial^{\beta} C}{\partial t^{\beta}}=-\frac{\partial C}{\partial X}+\frac{1}{Pe}\frac{\partial}{\partial X}\left(\frac{\partial^{\alpha} C}{\partial X^{\alpha}}\right), \tag{5}$$

$$\frac{\partial^{\lambda} C_1}{\partial t^{\lambda}}=\frac{\partial}{\partial Y}\left(\frac{\partial^{\zeta} C_1}{\partial Y^{\zeta}}\right) \tag{6}$$

where, C is the nondimensional concentration; X the spatial coordinates; t the nondimensional time; and Pe a Peclet number. The order of fractional derivative β predicts diffusion into the surrounding rocks. Above equations were differentiated by using binomial theorem, prior to the numerical calculations. Equation (5) and (6) are described by the Caputo fractional derivative; the concentration C is replaced by U (Chiba *et al*.(2006)).

As a result, equation (5) can be converted into the following form.

$$\frac{(U+C_0)_j^{n+1}-(U+C_0)_j^{n}}{\Delta t}+\sum_{k=0}^{n+1}\left(\frac{b}{(\Delta t)^{\gamma}}G_k^{\gamma}+\frac{1}{(\Delta t)^{\beta}}G_k^{\beta}\right)(U+C_0)_j^{n-(i-1)}=\frac{1}{\Delta X}(\tilde{f}_{j+1/2}^{n+1}-\tilde{f}_{j-1/2}^{n+1})-\frac{1}{Pe}\frac{1}{(\Delta X)^{\alpha+1}}\sum_{i=0}^{j+1}G_i^{\alpha}U_{j-(i-1)}^{n+1} \tag{7}$$

Here,

$$G_i^{\alpha}=\frac{\Gamma(-(\alpha+1)+i)}{\Gamma(-(\alpha+1))\Gamma(i+1)} \tag{8}$$

$$G_k^{\beta}=\frac{\Gamma(-\beta+k)}{\Gamma(-\beta)\Gamma(k+1)} \tag{9}$$

$$G_k^{\gamma}=\frac{\Gamma(-\gamma+k)}{\Gamma(-\gamma)\Gamma(k+1)} \tag{10}$$

$$(i=0,1,2,\cdots,j+1,\quad k=0,1,2,\cdots,n+1)$$

where, f is a numerical flux; C_0 is a concentration at $X = 0$. Advection term was differentiated by using the Total Variation Diminishing(TVD) scheme(Yee and Harten(1987)).

Similarly, equation (6) can be described as follows;

$$\frac{1}{(\Delta t)^{\lambda}}\sum_{k=0}^{n+1}G_k^{\lambda}(U_1+1)_j^{n-(k-1)}=\frac{1}{(\Delta Y)^{\zeta+1}}\sum_{i=0}^{j+1}G_i^{\zeta}U_{1\,j-(i-1)}^{\,n+1} \tag{11}$$

Here,

$$G_i^{\zeta}=\frac{\Gamma(-(\zeta+1)+i)}{\Gamma(-(\zeta+1))\Gamma(i+1)} \tag{12}$$

$$G_k^{\lambda}=\frac{\Gamma(-\lambda+k)}{\Gamma(-\lambda)\Gamma(k+1)} \tag{13}$$

$$(i=0,1,2,\cdots,j+1,\quad k=0,1,2,\cdots,n+1)$$

Results

The results of numerical simulations are shown in Figures 2 and 3 along with the analytical solutions. In the aquifer, the boundary conditions were as follows;

$$\begin{aligned}&C(X,0)=0,\\&C(0,t)=1,\\&C(\infty,t)\to 0.\end{aligned} \tag{14}$$

In the surrounding rocks, the boundary conditions were;

$$\begin{aligned}&C_1(Y,0)=0,\\&C_1(0,t)=1,\\&C_1(\infty,t)\to 0.\end{aligned} \tag{15}$$

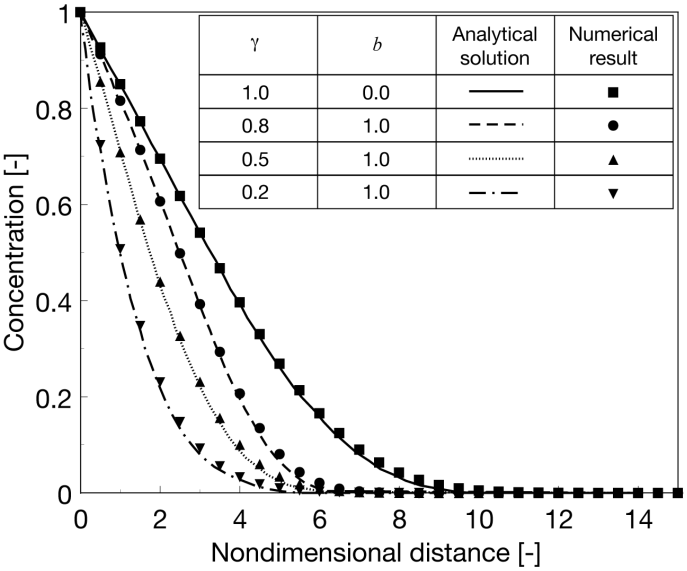

Figure 2. Comparison of the numerical and analytical solutions (fractured porous aquifer, α = 1.0, β = 0.5, *Pe* = 100, *t* = 15).

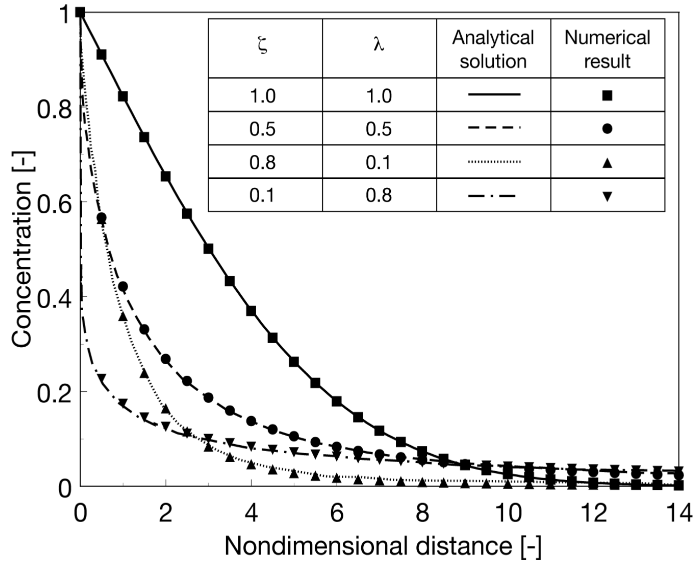

Figure 3. Comparison of the numerical and analytical solutions (surrounding rocks, *t* = 10).

All results are already converted to the non-dimensional form. In the Figures 2 and 3, the data points show the numerical results, and the continuous lines represent the analytical solutions. It is demonstrated that the numerical results agree well with the analytical solutions for several values of difference coefficients.

Conclusion

In this study, the reliable numerical algorithm for solving fractional differential equations is developed. And also, a numerical simulation method based on the Caputo fractional derivative was developed using binomial theorem and considering the initial values. The accuracy of numerical method is validated by comparison with exact analytical solutions available for some particular cases. Numerical results are in good agreement with their analytical solutions for several differential coefficients.

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