The Non-Fickan Effects of the Advection Diffusion on the Contaminants Transport in Porous Medium

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ABSTRACT

The transport equation of contaminants in a porous medium is usually described by parabolic convection diffusion differential equations. The implicit infinite velocity of propagation is apparently contrary to the reality of mass transport. In this paper, based on the modified Fick's law of non-equilibrium transmission, a hyperbolic convection diffusion differential equation is established, and the analytical solution of the concentration distribution of the pollutant transport in the half space is given. Numerical results show that the concentration distribution of contaminants from hyperbolic convective diffusion equation is limited in finite time, and the contaminant transport speed is limited. When the convection velocity is lower than the diffusion velocity, the concentration is reduced from the surface to the interior; while the convection velocity is greater than the diffusion velocity, the concentration distribution increases to the interior.1

INTRODUCTION

The migration of pollutants in porous media (e.g. soils, aquifers, plants and animals) is very complex, especially in aquifers. Many factors involve the migration of pollutants in the aquifer, such as temperature, pH, concentration of pollutants, pollutant composition, microbial activity and plant absorption, porous medium in homogeneity and anisotropy, and rock cracks, joints and faults, karst pipes etc. The migration and transformation of pollutants in porous media of rock and soil mainly occur water rock interaction with rock medium, which mainly include physical

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process, chemical process and biological process. The physical processes include convection, diffusion and dispersion, physisorption and desorption, and chemical processes include chemisorption and desorption, dissolution and precipitation, redox, and so on.

The transport of pollutants in porous media involves complex processes, and classical one dimension advection diffusion equations (ADE) are usually used

\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}
\]  

(1)

Where \( C \) = the contaminant concentration, \( D \) = the dispersion coefficient, \( u \) = the average fluid velocity, \( x \) = position, and \( t \) = time. The ADE formulation holds two main assumptions: that the center of mass of the contaminant plume travels with the average (‘’macroscopic’’) fluid velocity and that the mechanical and chemical spread of the contaminant around this center of mass can be described completely by a Fickian process. Although the ADE equation contaminant has passed through a relatively small heterogeneous medium, it has been successful. But in many cases, the ADE equation cannot describe the migration of pollutants in heterogeneous media[1].

From the mathematical point of view, equation (1) is parabolic convection diffusion equation, the contaminants transfer in the porous media results from convection and diffusion mechanism, the speed of propagation of material concentration is infinity on the Eq.(1). This is clearly paradox with physical reality[4]. However, A large number of experiments show that the velocity of mass diffusion is not infinite, and the defects of Eq.(1) is attributes to Fick law included in Eq.(1)[2,3,4].

In the past decades, the modified Fick's law or Fourier law is proposed by Cattaneo who presented a generalization of Fourier’s law that overcomes the infinite speed paradox[5,6,7]. This paper established the hyperbolic advection dispersion equation of Fick's law to investigate contaminants transport. Considering the half space with surface constant concentration, a mathematical model is built and the theoretical solution is derived, The comparison differences of the numerical results of classical convection dispersion and non-Fick’s law of diffusion convection,

MATHEMATICAL MODELING

One-dimensional convection and dispersion of contaminants occurring in porous media are considered here. Concentrations \( C_0 \) of contaminants are continuously injected at the beginning of the semi-infinite cylindrical porous medium at the beginning of the aquifer, and the concentration differences of contaminants in different convection diffusion equations at any given time are sought. It is assumed that the initial contaminants in the aquifer is zero everywhere,
the seepage is homogeneous, the dispersion is one-dimensional, and the contaminants in the aquifer are passive without sinks.

For the contaminants transportation in porous medium, one dimension continuous equation of the convective diffusion is

$$\frac{\partial C}{\partial t} n = -\frac{\partial J}{\partial x}$$  \hspace{1cm} (2)

where n = porosity; J = mass flux.

Considering the following constitutive relation with non-equilibrium process [8]

$$J = \frac{1}{\xi} \int_{0}^{\xi} \exp \left(-\frac{t - \tau}{\xi}\right) \left(-D \frac{\partial C}{\partial x} + UC\right) d\tau$$ \hspace{1cm} (3)

The hyperbolic advection diffusion equation is derived inserting Eq.(2) into Eq.(3)

$$\frac{\partial \bar{C}}{\partial t^2} + \frac{\partial \bar{C}}{\partial t} + D \frac{\partial^2 \bar{C}}{\partial x^2} - U \frac{\partial \bar{C}}{\partial x} = 0$$ \hspace{1cm} (4)

The initial condition is assumed as

$$C(x, t) = 0 \quad \frac{\partial C}{\partial t} = 0 \quad t = 0$$ \hspace{1cm} (5)

The boundary condition is defined as

$$C(x, t) = C_0 \quad x = 0$$ \hspace{1cm} (6)

$$C(x, t) = 0 \quad x \rightarrow \infty$$ \hspace{1cm} (7)

**SOLVING**

Following dimensionless quantities are introduced

$$\phi = \frac{C}{C_0}, \quad \eta = \frac{x}{\sqrt{D\tau}}, \quad \xi = \frac{t}{\tau}, \quad u = \frac{U}{\sqrt{D/\tau}}$$ \hspace{1cm} (8)

Inserting Eq.(10) into Eq.(4), (7), (8), (9), following dimensionless equation are derived
\[
\frac{\partial^2 \phi}{\partial \zeta^2} + \frac{\partial \phi}{\partial \xi} = \frac{\partial^2 \phi}{\partial \eta^2} - u \frac{\partial \phi}{\partial \eta} \tag{9}
\]

\[
\phi(\eta, \xi) = 0, \quad \frac{\partial \phi}{\partial \xi} = 0 \quad \xi = 0
\tag{10}
\]

\[
\phi(\eta, \xi) = 1 \quad \eta = 0
\tag{11}
\]

\[
\phi(\eta, \xi) = 0 \quad \eta \to \infty
\tag{12}
\]

Applying Laplace transformation to Eq.(9), Transformed equation is given as

\[
\frac{\partial^2 \bar{\phi}}{\partial \eta^2} - u \frac{\partial \bar{\phi}}{\partial \eta} - (s + 1) \bar{\phi} = 0
\tag{13}
\]

\[
\bar{\phi}(\eta, s) = \frac{1}{s} \eta = 0
\tag{14}
\]

where

\[
\bar{\phi}(\eta, s) = \int_0^\infty \exp(-st)\phi(\eta, t)dt
\]

the solution of the Eq.(12) is derived as

\[
\bar{\phi} = \frac{1}{s} \exp\left(\frac{u}{2} \eta\right) \exp\left(-\eta \sqrt{\frac{u^2}{4} + s(s + 1)}\right)
\tag{15}
\]

The inverse Laplace transformation of Eq.(15) is written as

\[
\phi(\eta, \xi) = \exp\left(\frac{u}{2} \eta\right) \exp\left(-\frac{\xi}{2}\right) f_i(\eta, \xi)
\tag{16}
\]

In the case of \( u > 1 \)

\[
f_i(\eta, \xi) = \begin{cases} 
0 & \eta < \xi < \eta \\
\exp\left(-\frac{\eta}{2}\right) + \sqrt{\frac{u^2 - 1}{2}} \eta \int_{\frac{\xi}{\sqrt{\eta^2 - \xi^2}}}^{\frac{\eta}{\sqrt{\eta^2 - \xi^2}}} d\tau & \xi > \eta
\end{cases}
\tag{17a}
\]

In the case of \( 0 < u < 1 \)
\[
f_i(\eta, \xi) = \begin{cases} 
0 & \xi < \eta \\
\exp\left(-\frac{\eta}{2}\right) + \frac{1}{\sqrt{\tau^2 - \eta^2}} \int_0^\tau \frac{1}{\sqrt{\tau^2 - \eta^2}} d\tau & \xi > \eta 
\end{cases}
\]  \quad (17b)

In the case of \( u = 1 \)

\[
f_i(\eta, \xi) = \begin{cases} 
0 & \xi < \eta \\
\exp\left(-\frac{\eta}{2}\right) & \xi > \eta 
\end{cases}
\]  \quad (17c)

If the non-Fickan effects is ignored, the classical solution of the same problem is derived

\[
\phi(\eta, \xi) = \exp\left(\frac{u}{2}\right) \exp\left(-\frac{u^2}{2}\right) \int_0^\xi \exp\left(-\frac{u^2}{2}\right) d\tau
\]  \quad (18)

**CALCULATION AND DISCUSSION**

In order to eliminate the defects of the traditional convection dispersion equation, the hyperbolic convection dispersion model is built based on non-equilibrium Fick law and the theoretical solution of problem is given. On the solutions of Eq.(18) and Eq.(20), the numerical comparison results are shown in figures 2 and 3 to compare different mechanism of contaminants transfer in porous medium.

![Figure 1. Comparisons of concentration distribution on u=0.5.](image-url)
Fig. 1 and Fig. 2 show the different mechanism of contaminant transfer. Compared to the results from the Eq. (20), concentration distribution zones from the Eq. (18) is finite. When the dimensionless time is 0.3, the concentration distribution range is not more than 0.3. This is attributed to the hyperbolic advection diffusion equation. However, classical advective diffusion equation imply infinite diffusion velocity.

From the definition of dimensionless \( u = \frac{U}{\sqrt{D/\tau}} \). The ratios indicate the effects of two mechanisms of convection and dispersion on contaminant concentration transport. \( u < 1 \) means diffusion transport occupying a dominant position. The concentration is lowered from the surface to the interior in Fig. 1. However, \( u > 1 \) means advection transport occupying a dominant position, The concentration distribution increases to the interior in Fig. 2.

CONCLUSIONS

Numerical results show that the concentration distribution of contaminants from hyperbolic convective diffusion equation is limited in finite time, and the contaminant transport speed is limited. When the convection velocity is lower than the diffusion velocity, the concentration is reduced from the surface to the interior; while the convection velocity is greater than the diffusion velocity, the concentration distribution increases to the interior.
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REFERENCES