Explicit Finite Difference Solution for One Dimensional Solute Transport of Unstable Flow

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ABSTRACT

Research on solute transport of unstable flow is of great significance for industrial and agricultural production, management and controlling of water resource, environmental protection and administration as well as restoration of nuclear rubbish. Furthermore, solute transport of unstable flow is quite more general than solute transport of constant flow in practice of industrial and agricultural production. Based on traditional time domain difference methods, this work calculated the one-dimensional solution transport problem of unstable flow by adopting explicit difference method. The validation of computational method is verified by analyzing the results. And then a conceptual knowledge of solute transport behavior of unstable flow is acquired. This indicates the method presented is of high validity, efficiency and accuracy and is suitable for more complicated modelling. Furthermore, the numerical analysis methods presented can be applied for 2-D and/or 3-D solute transport of unstable flow for modelling and prediction of complicated solute movement process.¹

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KEYWORDS


INTRODUCTION

The study on the transport law of soil solute is of great significance for soil salt and alkali, soil and fertilizer utilization, production of industrial and mineral industry and the discharge of pollutants caused by rainwater runoff and geological storage of nuclear waste [1-5]. The solute dissolved in the groundwater can not only move with the groundwater, but also diffuse as the diffusion movement of water molecules. Therefore, the soil solute transport model is composed of the problem of groundwater flow and the solute transport. Solution of solute transport requires simultaneous solution of water flow problem and solute transport problem. For problems like the safety assessment of geological storage of nuclear wastes, groundwater pollution and the design of remediation, it is necessary to predict the flow of groundwater and the transport of contaminated materials in large space and long time span. There are many methods for determining the solutions such as finite difference method, finite element method, boundary element method and finite analysis method. Among these numerical solutions, the finite difference method is the most widely used for its simplicity and clear physical meaning and so on. Compared with the extensive attention of the steady flow solute transport, the study on the solute transport of unsteady flow is almost blank in China[1,3]. In this paper, a numerical formula of the explicit time domain difference method for one dimensional solute transport is established for the first time. The temporal and spatial distribution of solute concentration is calculated and the results are qualitatively analyzed.

BASIC PRINCIPLE

According to Shao[1], the basic equations of solute transport for unsteady flow parameters of solute transport are

$$\frac{\partial (\theta c)}{\partial t} = \frac{\partial}{\partial x} \left( D(c) \frac{\partial c}{\partial x} \right) - \frac{\partial (qc)}{\partial x} \frac{\partial \theta}{\partial t} = - \frac{\partial q}{\partial x} \frac{\partial \theta}{\partial x} + \mathcal{K}(\theta)$$

(1)

The conditions of solution are

$$c(x,0) = c_i, \quad \theta(x,0) = \theta_i, x \geq 0, t = 0$$

(2)

$$c(0,t) = c_0(t), \quad \theta(0,t) = \theta_0(t), x = 0, t \geq 0$$

(3)
\[ c(l, t) = c_i, \quad \theta(l, t) = \theta_i, \quad x = l, t \geq 0 \]  \hspace{1cm} (4)

Where \( x \) is the length coordinates of the flow direction, \( t \) is time, \( c = c(x, t) \) is the concentration of solute in the flow, \( \theta = \theta(x, t) \) is the water content in the soil, \( l \) is the amount of water in the soil, \( c_i \) is the initial solute concentration in the flow, \( \theta_i \) is the initial water content in the soil, \( c_0(t) \) is the concentration of the solute in the water at \( x = 0 \), \( \theta_0(t) \) is the water content in the soil at \( x = 0 \), \( q \) is the velocity of water and \( \overline{D(c)} \) the diffusivity of the solute in the water. \( D(\theta) \) is the diffusion coefficient of soil water, \( K(\theta) \) is the soil water conductivity. Assuming that [1]

\[
D(\theta) = \frac{k_s}{ab(\theta_s - \theta_i)} \Theta^{2+1/b}; \quad K(\theta) = k_s \Theta^{3+2/b}; \quad \Theta = \frac{\theta - \theta_i}{\theta_s - \theta_i}; \quad \overline{D(c)} = D_0 e^{\beta c} \]  \hspace{1cm} (5)

Where \( \Theta \) is dimensionless water content, \( \theta_s \) and \( \theta_i \) saturation value and residual value of soil volumetric water content, \( k_s \) saturated hydraulic conductivity and \( a, b \) and \( \beta \) are model parameters.

**THEORY AND FORMULATION**

Because water content and solute concentration vary with time and space. The finite length \( l \) of water flow can be taken along the \( x \) direction as the calculation object, and it will be divided into \( n \) element with equal distance, each node is numbered by \( i, i = 0, 1, 2, \ldots, n \), with the step length \( \Delta x = l/n \), the time coordinate is divided into time step \( \Delta t \), and the node is numbered by \( k, k = 0, 1, 2, \ldots, m \).

The difference equations of the equations (1) at any inner node are then obtained as following[1]

\[
\frac{\theta_i^{k+1} - \theta_i^k}{\Delta t} = \frac{D_{i+1/2}^k (\theta_{i+1}^k - \theta_{i}^k) - D_{i-1/2}^k (\theta_{i}^k - \theta_{i-1}^k)}{\Delta x^2} - \frac{K_{i+1}^k - K_{i-1}^k}{2\Delta x} \]  \hspace{1cm} (6)

\[
\frac{(\Delta c)^{k+1} - (\Delta c)^k}{\Delta t} = \frac{\overline{D_{i+1/2}}^k (c_{i+1}^k - c_{i}^k) - \overline{D_{i-1/2}}^k (c_{i}^k - c_{i-1}^k)}{\Delta x^2} - \frac{(qc)_{i+1}^k - (qc)_{i-1}^k}{2\Delta x} \]  \hspace{1cm} (7)

\[
q_i = -\frac{D_i (\theta_{i+1} - \theta_{i-1})}{2\Delta x} + K_i \]  \hspace{1cm} (8)
Differential progressive scheme can be obtained by deformation of formula (6)

\begin{equation}
\theta_i^{k+1} = rD_i^{k+1/2}\theta_i^k + \left(1 - rD_i^{k+1/2} - rD_i^{k-1/2}\right)\theta_i^k + rD_i^{k-1/2}\theta_{i-1}^k - \gamma K_{i+1}^k + \gamma K_{i-1}^k
\end{equation}

(9)

\begin{equation}
\left(\alpha c\right)_i^{k+1} = \left(\alpha c\right)_i^k + rD_{i+1/2}c_{i+1}^k - r\left(D_{i+1/2} + D_{i-1/2}\right)c_i^k + rD_{i-1/2}c_{i-1}^k - \gamma (qc)_i^k + \gamma (qc)_i^{k-1}
\end{equation}

(10)

Where

\begin{equation}
D_{i+1/2}^k = \frac{1}{2}\left(D_i^k + D_{i+1}^k\right); \quad D_{i-1/2}^k = \frac{1}{2}\left(D_i^k + D_{i+1}^k\right)
\end{equation}

(11)

\begin{equation}
D_{i+1/2}^k = \frac{1}{2}\left(D_{i+1}^k + D_i^k\right); \quad D_{i-1/2}^k = \frac{1}{2}\left(D_{i+1}^k + D_i^k\right)
\end{equation}

(12)

The above difference equation can be used to calculate the water content and solute concentration in each time period at each node. Since the values of \(c\), \(\theta\) and its corresponding values of \(\overline{D}(c)\), \(D(\theta)\) at the initial time \(t = 0\) and boundary 
\(Z = 0, l\) are known, \(c_0^k\), \(\theta_0^k\), \(D_0^i\) and \(\overline{D}_0^i\) \(i = 0, 1, 2, \ldots, n\) and \(c_n^k\), \(c_n^k\), \(\theta_n^k\), \(D_n^k\),
\(D_n^k\) and \(\overline{D}_n^k\) \(k = 0, 1, 2, \ldots, m\) can also be known. The computation can start
from the first period of time \(k = 1\). And for each time period, only \(n\) nodes of
\(i = 1, 2, \ldots, n - 1\) were computed. The explicit procedure can be recurred in this
work.

**CALCULATION RESULTS AND DISCUSSION**

According to the algorithm presented in section 2, a program has been
completed in FORTRAN language to obtain the distribution of water, solute
concentration and other parameters along the soil depth for investigation of law of
solute transport and the reliability of the numerical algorithm in the unsteady flow
with changing solute transport parameters. The model parameters used in the
example are as follows, \(\theta_i = 0.11\), \(\theta_0 = 0.376826\), \(l = 5\), \(a = 0.6578\),
\(b = 1.036\), \(\theta_s = 0.49\), \(\theta_r = 0.03\), \(k_s = 0.85895 \times 10^{-3}\), \(D_0 = 0.31 \times 10^{-6}\),
\(\beta = 5.0\), \(c_i = 0.11\), \(c_0 = 0.5\), \(t_0 = 6 \times 10^5\), \(\Delta t = 10\). The distribution of water
along the soil depth at \(t = 30000, 60000, 120000, 150000, 240000, 500000\) and
420000 seconds at different times is shown in Figure 1. It is easy to see that water
wetting front is obvious in this case of water conductivity model and its
parameters.
Figure 2 shows the distribution of solute concentration along the soil depth at $t=30000$, 60000, 120000, 150000, 240000, 300000, 420000, 600000 seconds at different times. Compared with the constant water velocity and the constant water content, the distribution mode of the solute concentration is different from the condition of variable water velocity and water content. Relatively, due to the movement of water in the upper layer of soil the velocity of solute transport is faster at the initial time, and the distribution pattern of solute concentration along the soil depth in $t=30000$ seconds is different from that in $t=300000$, 420000 and 600000 seconds.

Figure 3 shows the distribution of solute content along the soil depth at time $t=30000$, 60000, 120000, 150000, 240000, 300000, 420000, 600000 seconds at different times. It can be seen from the figure that the velocity of solute diffusion is faster than the velocity of water migration, and the content of solute shows an obvious three segment distribution pattern in the initial period until time $t=240000$, and at time $t=300000$ and 420000 seconds change to two segment pattern, and finally at time $t=600000$ seconds change to one segment pattern.
Figure 4 shows the distribution of water movement velocity along the soil depth at different time $t=30000$, $60000$, $120000$, $150000$, $240000$, $300000$, and $420000$ seconds. It can be seen from the figure that the velocity of soil moisture movement in the initial time shows a distinct distribution pattern with variation from large to small along the soil depth. With time increasing, the speed of movement gradually change to a uniform pattern from the outside to the inside.

Figure 5 shows that the soil moisture diffusion coefficient varies with soil depth at different time $t=30000$, $60000$, $120000$, $150000$, $240000$, $300000$ and $420000$ seconds. It can be seen from the figure that the change of soil moisture diffusion coefficient with soil depth is very similar to change of water with soil depth as shown in Figure 1.

Figure 6 shows that the diffusion coefficient of solute in soil varies with soil depth at different time $t=30000$, $60000$, $120000$, $150000$, $240000$, $300000$ and $420000$ seconds. From the figure, it can be seen that the solute concentration curves smoothly vary with the soil depth, and the solute diffusion coefficient also smoothly vary with the soil depth.

Figure 7 shows the variation of soil water conductivity with soil depth at different time $t=30000$, $60000$, $120000$, $150000$, $240000$, $300000$ and $420000$ seconds. The change of soil water conductivity with soil depth and the variation of soil moisture with depth of soil shown in Fig. 1 and the variation of soil moisture diffusion coefficient with soil depth shown in Figure 5 are similar. It is
this similarity that reflects the consistency of soil water movement and the correctness of the calculation results.

CONCLUSIONS

The explicit difference algorithm and processing technique presented in this work is suitable for more complex models and can be applied to areas of industry, agriculture, resources and environment and extended to the prediction and simulation of the solute migration in groundwater systems ranging from tens to hundreds of kilometers in space and from thousands to tens of thousands of years.

ACKNOWLEDGEMENTS

This work was financially supported by the Foundation for Hunan Provincial Key Disciplines of the 13th Five-Year Plan.

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