Journal of Zhejiang University SCIENCE
ISSN 1009-3095
http://www.zju.edu.cn/jzus
E-mail: jzus@zju.edu.cn

Combinatorial model of solute transport in porous media*

ZHANG Miao-xian (张妙仙)[1], ZHANG Li-ping (张丽萍)[2]

([1]*College of Engineering, Zhejiang Forestry University, Lin'an 311300, China*)

([2]*Institute of Soil and Water Resources and Environmental Science, College of Environmental and Resource Science, Zhejiang University, Hangzhou 310029, China*)

E-mail: zhangmx18@163.com; lpzhang@zju.edu.cn

Received Sept. 26, 2003; revision accepted Mar. 8, 2004

Abstract: Modeling of solute transport is a key issue in the area of soil physics and hydrogeology. The most common approach (the convection-dispersion equation) considers an average convection flow rate and Fickian-like dispersion. Here, we propose a solute transport model in porous media of continuously expanding scale, according to the combinatorics principle. The model supposed actual porous media as a combinative body of many basic segments. First, we studied the solute transport process in each basic segment body, and then deduced the distribution of pore velocity in each basic segment body by difference approximation, finally assembled the solute transport process of each basic segment body into one of the combinative body. The simulation result coincided with the solute transport process observed in test. The model provides useful insight into the solute transport process of the non-Fickian dispersion in continuously expanding scale.

Key words: Modeling, Mass transport, Expanding scale, Combinatorics
Document code: A **CLC number:** X144

INTRODUCTION

In recent years, modeling of solute transport in porous media remains a key issue in the area of soil physics and hydrogeology, because anthropogenic chemicals frequently enter the soil, subsoil and aquifers, either by accident or by accepted management practices, and the resulting chemical residues pose hazards to the environment.

The movement of solute in porous media is commonly described by the convection-dispersion equation (CDE) (Bear, 1972) developed and extensively applied to predict the contamination transport (Bresler, 1981; Van and Shouse, 1989). The CDE is a differential equation for dealing with the complexity of the distribution and change of pores velocities in porous media, and conveniently describing the solute transport through porous media and is based on three basic assumptions: assumption of porous continuous media, assumption of average flow velocity, and assumption of Fick's first law for solute dispersion; and describes solute transport as the sum of the average convection with flow, and the hydrodynamic dispersion (Lei *et al.*, 1988; Li and Li, 1998).

However, the CDE results in scale-dependent dispersion. The most important drawbacks of CDE when it is used to simulate solute transport, can be attributed to the non-Fickian behavior of dispersive transport as well as the apparent scale dependence of the dispersivity (Huang, 1991; Cyril and van der Lee, 2001). So people have continuously been exploring new theories and methods to study the sol-

*Project supported by the National Basic Research Program (973) of China (No. G1999011803), and the Main Research Direction of Knowledge Innovating Projects from Academy Sinica (No. KZCX3-SW-428)

ute transport process in porous media. Different theories have been proposed to explain and to express hydrodynamic dispersion in porous media.

Stochastic theory was extensively applied firstly (Yang *et al.*, 2000; Zhang, 2001). Some typical stochastic models were presented: random walk model (Cyril and van der Lee, 2001), scaling theories (Nielsen *et al.*, 1973; Lei *et al.*, 1988; Neuman, 1990), stream tube model (Toride and Leij, 1996), transfer function model (Jury *et al.*, 1986), double velocity model (Grubert, 1999), automation model (Yang *et al.*, 1998a), continuous time random walk (Briam *et al.*, 2000), etc. In the stochastic models, soil porous media was taken as stochastic media, solute transport process was described as stochastic process (Yang *et al.*, 1998b), so that they could not explain the physics mechanism of solute transport.

However, porosity, incompactness, and combinatorial characteristics are the basic characteristics of soil determined by sediment regulation and cultivation. Solute particles transport continuously with the water flow in the soil pores. Because of the restraining pores, the velocities, directions and routes of solute particles movement change continuously; solute flows in soil pores merge and divide frequently, leading to solute dispersion. To resolve the solute transport problem in porous media, it is necessary to describe the combining and distributing rules of soil pores and the solute transport process by appropriate mathematical methods.

Combinatorics is a mathematical method for arranging some discrete units according to certain regulation (Qu, 1989). Combined algorithm is one of the most important algorithms in computer science nowadays. Combinatorics principles can perfectly deal with the dispersive and combinatorial characteristics of solute transport in porous media. A combinatorics model can really reflect solute transport process in porous media.

COMBINATORICS MODEL

To study solute transport on the basis of combinatorics, the actual soil porous media is first regarded as an assemblage body of many "basic segments". Then after the solute transport process of each "basic segment" is determined, the solute transport process of combination body is determined by combinatorial method.

Solution concentration equations

Suppose water solution from steady or temporary pulse source and at concentration is c_1, infiltrates through soil column with cross-sectional area A and where the initial solution concentration is c_2. Again we consider the soil as inert, ignoring its molecular diffusion. And suppose that the velocity of the porewater is known, that the maximal porewater velocity is $V_{\max}$, that the minimal porewater velocity is $V_{\min}$, and $V(i)$ is the porewater velocity at (i). The area of soil porous to $V(i)$ is $a(i)$ and that the ratio of $a(i)$ in the total soil pores section area is $p(i)$.

For certain column, we can determine the breakthrough curve of solute transport by mixed displacement experiments. The relative concentration of discharged solution, $(c-c_2)/c_1$, is actually the ratio $p(i)$ at certain time. That is:

$$\sum_{V=\frac{L}{t}}^{V_{\max}} p(i) = \frac{c-c_2}{c_1} \tag{1}$$

On the basis of the assumptions mentioned above, we discuss the respectively solute transport processes under steady source and pulse source.

(1) Solution concentration equations on condition of steady source

At time t, and at the position L from the infiltration inlet section of the soil column, the concentration c of the soil solution is:

$$\begin{cases} c = c_1 & 0 \le L \le tV_{\min} \\ c = c_1 \sum\limits_{V=\frac{L}{t}}^{V_{\max}} p(i) + c_2 \sum\limits_{V_{\min}}^{V=\frac{L}{t}} p(i) & tV_{\min} < L < tV_{\max} \\ c = c_2 & L \ge tV_{\max} \end{cases} \tag{2}$$

(2) Solution concentration equations on con-

dition of pulse source

When the pulse time is T, and $t>T$, then at time t, at the position L from the infiltration inlet section, the concentration c of the soil solution is:

$$\begin{cases} c=c_2 & 0\le L\le (t-T)V_{\min} \\ c=c_1\sum_{V=\frac{L}{t}}^{V=\frac{L}{t-T}} p(i)+c_2[1-\sum_{V=\frac{L}{t}}^{V=\frac{L}{t-T}} p(i)](t-T) & V_{\min}<L<tV_{\max} \\ c=c_2 & L\ge tV_{\max} \end{cases} \quad (3)$$

The length of the dispersion band is $L_d=V_{max}t-V_{min}(t-T)$. Generally, $V_{min}\times T$ is fairly small, so $V_{min}\times T$ can be ignored, that is:

$$L_d=(V_{max}-V_{min})t \quad (4)$$

Assembling model

As the length of solute transport distance increase, the available transport paths of solute particles increase, and the chances and frequency of embranchment and combination of pore's flow increase. Pores flow velocities also change with time and distance. The next key problem is how to determine the changes of pores flow velocities with time and distance. Suppose the meeting opportunity of different pore's flows is equal. According to the combinatorics principle, we can assemble pore's flows together.

The assembled model is:

$$\begin{cases} V(j)=\dfrac{V(i)+V(k)}{2} \\ p(j)=p(i)p(k) \\ a(j)=\dfrac{[a(i)+a(k)]}{2} \end{cases} \quad (5)$$

where, i, k is grouping order of pore's flow velocities in successional segments respectively; j is grouping order of pore's flow velocities after i is combined with k.

COMPUTER SIMULATION

According to the principles mentioned above, first, we must obtain $p(i)$, and $V(i)$ and $a(i)$ of each segment by difference approximation for the solute breakthrough curve. Then, according to the Eq.(5), we can work out the $p(j)$, and $V(j)$ and $a(j)$ of j segment which is the accumulative total of i segment and k segment. Again, introduce the $p(j)$, and $V(j)$ and $a(j)$ into the Eqs.(1)–(3). So we obtain the solute concentration distribution in the length of j segment. As the length of the segment is continually increased, and new $p(j)$, and $V(j)$ and $a(j)$ are continually obtained, the processes go on again and again, and the solute transport process can be described.

Table 1 shows that the main characteristic values of solute transport by computer simulation, when the solute transport distance was 1 L, 2 L, 4 L, 8 L. Computer simulation yielded the following results:

1. Without regard the particle's velocity discrepancy, infiltration for water flow can be studied by macrocosmic method. However, we must consider the particle's velocity discrepancy in order to get the variation of the solution concentration in studying solute transport.

2. With the increase of transport distance, the dispersion zone will lengthen, the concentration of the dispersion zone will be gradually diluted and the kurtosis of the solution's concentration distribution will gradually level off. The results of hydrodynamic dispersion are that the solution concentration and background concentration come equal. The simulation result coincided with the solute transport process observed in test.

Table 1 Main eigenvalues of solute transport with lengthening distance

Relative distance	Relative dispersion peak concentration	Relative position of dispersion peak	Minimal relative transport distance	Relative width of dispersion zone
1	0.460	0.714	0.571	0.429
2	0.330	1.714	1.143	0.857
4	0.151	3.114	2.286	1.714
8	0.088	6.286	4.571	3.429

CONCLUSION

Combination and incompactness are the basic characters of soil. For these reasons, the article applied combinatorics principle to solute transport in porous media and suggested a solute transport model in continuously expanding scale. The combinatorics model regarded actual porous media as a combinative body of many basic segments. We studied the solute transport process in each basic segment of soil body, and assembled the solute transport process of each basic segment of soil body into the solute transport process of the combinative body. The velocity distribution of solute transport of each basic unit of soil body was deduced from the solute breakthrough curve by difference approximation. We simulated respectively the solute transport processes under steady source and pulse source by computer. The simulation result showed that the model is more suitable for describing the solute transport process in continuously expanding scale than the traditional convection-dispersion equation. It is a new way to apply the results obtained in laboratory to the field, and an important breakthrough in solving the problem of soil solute transport in different scales.

References

Bear, J., 1972. Dynamics of Fluid in Porous Media. American Elsevier, New York.

Bresler, E., 1981. Transport of salts in soils and subsoils. *Agric. Water Management*, (4):35-62.

Briam, B., Harvey, S., Stephen, E.S., 2000. Anomalous transport in laboratory-scale, heterogeneous porous media. *Water Resour. Res.*, **36**(1):149-158.

Cyril, F., van der Lee, J., 2001. A stochastic model of transport in three-dimensional porous media. *Mathematical Geology*, **33**(4):449-474.

Grubert, D., 1999. Effective parameter interpretation and extrapolation of dispersion simulations by means of a simple two-velocity model. *Transport in Porous Media*, **37**:153-167.

Huang, K.L., 1991. Scale-dependence of hydrodynamic dispersion in porous media. *Hydrogeology and Engineering Geology*, (3-4):25-33 (in Chinese).

Jury, W.A., Sposito, G., White, R.E., 1986. A transfer functions model of solute transport through soil 1. Fundamental concepts. *Water Resour. Res.*, **22**(2): 234-247.

Lei, Z.D., Yang, S.X., Xie, S.C., 1988. Hydrodynamics in Soil. Tsinghua University Press, Beijing, China, p.203-260 (in Chinese).

Li, Y.Z., Li, B.G., 1998. Solute Transport in Soil. Science Press, Beijing, China, p.113-152 (in Chinese).

Neuman, S.P., 1990. Universal scaling of hydraulic conductivity and dispersivities in geological media. *Water Resour. Res.*, **26**(8):905-908.

Nielsen, D.R., Biggar, J.W., Erh, K.T., 1973. Spatial variability of field-measured soil-water properties. *Hilgardia*, **42**:215-259.

Qu, W.L., 1989. Combinatorics. Beijing University Press, China, p.33-54 (in Chinese).

Toride, N., Leij, F.J., 1996. Convective dispersive stream tube model for field scale solute transport: I moment analysis. *Soil Sci. Soc. AM. J.*, **60**:342-352.

Van, G.M.T., Shouse, P.J., 1989. Solute Transport in Heterogenous Field Soil. *In*: Allen, D.T., *et al.*(ed.). Intermedia Pollutant Transport. Plenum Publ. Corp., New York, p.177-187.

Yang, D., Udey, N., Spanos, T.J.T., 1998a. Automation simulations of dispersion in porous media. *Transport in Porous Media*, **32**:187-198.

Yang, J.Z. , Chai, S.Y., Ye, Z.T., 1998b. Study and advance about the stochastic theory of groundwater solute transport in region. *Hydrology Science Advance*, **9**(1): 85-98 (in Chinese).

Yang, J.Z., Chai, S.Y., Huang, G.H., Ye, Z.T., 2000. Stochastic Theory of Water and Solute Transport in Porous Media. Science Press, Beijing, China, p.129-156 (in Chinese).

Zhang, M.X., 2001. Information-statistics Evaluation on the Effect of Ground Water Buried Depth to Upper Soil and Ground Water Salinity. China Postdoctoral Preceding. Science Press, Beijing, China, p.221-224 (in Chinese).