Study on contaminant transport in one-layered media with variable diffusion coefficient

Chuang Yu i) , Junfeng Liu ii) and Jiangwei Xu iii)

i) Professor, College of Architecture and Civil Engineering, Wenzhou University, Zhejiang Wenzhou 325035, China.
ii) Master Student, College of Mathematics & Information Science, Wenzhou University, Zhejiang Wenzhou 325035, China.
iii) Master Student, College of Mathematics & Information Science, Wenzhou University, Zhejiang Wenzhou 325035, China.

ABSTRACT

With considering the distance-dependent diffusion coefficient, a one-dimensional contaminant diffusion model was developed. An analytical solution was obtained by using the orthogonal expansion method. The corresponding program was compiled on the basis of the proposed solution, and the effect of the relevant parameters on contaminant transport was analyzed. The results indicate that the diffusion coefficient has complex effects on the transport of contaminants. On one hand, the initial diffusion coefficient and heterogeneity parameter will affect the time of contaminant concentration reaches steady state, and on the other hand, the heterogeneity parameter affects the concentration of steady state. In addition, the influence of related parameters on the bottom flux of contaminant was discussed. The proposed analytical solution can be used for verification of complicated numerical models and experimental data fitting.

Keywords: contaminant, diffusion, variable diffusion coefficient, analytical solution

1 INTRODUCTION

Contaminant transport analysis is a hot research problem when considering geo-environmental problems such as the evaluation and design of the barrier systems for waste disposal and the remediation of existing contaminated sites. Studying the contaminant transport can effectively control the pollution problems caused by the leakage of pollutants. Mathematical model is a powerful tool for researching the contaminant transport, and is widely applied to the contaminant transport analysis (Singh, 2011).

Contaminant transport in the soil medium is influenced by many factors (Chen et al, 2012), such as advection, diffusion, adsorption, degradation, etc. The Chinese standard code for liner systems consisted of compacted clay requires the hydraulic conductivity less than $10^{-7} \text{ cm/s}$. In previous studies, the hydraulic conductivity is considered as the main process of contaminant transport in clay liners. But research showed that careful attention to construction procedures results in high quality clay liners having a hydraulic conductivity less than $10^{-7} \text{ cm/s}$ (Edil, 2003). For instance, clay liners in Wisconsin typically have very low field hydraulic conductivities, on the order of $10^{-6}$ cm/s. (Gordon et al, 1990; Benson et al, 1999).

Furthermore, investigations have shown that leachates do not have a detrimental impact on the hydraulic conductivity of compacted clay (Berger et al, 2002; Kalbe et al, 2002; Kim et al, 2003; Frempong, et al, 2008).

Research has also shown that contaminant diffusion (contaminant transport caused by the difference in concentration between the top and bottom of the liner) is often the dominant mode of contaminant transport in well-built liner systems (Toupiol et al, 2002; Willingham et al, 2004; Bezza et al, 2009). Many mathematical models can be solved by using numerical methods, such as the finite difference method, the boundary element method, and the finite element method. Analytical solution is an economical and effective method compared with numerical method, because they can provide better physical insights into the problems and are relatively more simplistic (Rowe et al, 1997; Xie et al, 2010; Guan et al, 2012). Liu and Ball (1998) presented the analytical solution for solute diffusion in a semi-infinite two-layer porous medium for arbitrary boundary and initial conditions. Shackelford et al (2005), Chen et al (2006), Li and Cleall (2010) have provided the analytical solutions for contaminant diffusion through finite multi-layered media under different boundary conditions.

However, all the above studies are undertaken with constant diffusion coefficient. Due to the heterogeneity of the medium, constant diffusion coefficient models often result a certain error. In recent years, many authors have pointed out that the diffusion coefficient is varying with distance or time. Wang et al (1996), Chen et al (2008), Pérez Guerrero et al (2010) and You et al (2013) have studied the model with variable diffusion
coefficient for different types, and obtained the analytical solution. The above variable diffusion coefficient models are relatively complicated, and difficult for practical application. This study will simplify the type of diffusion coefficient and simulate the contaminant transport.

In this paper, the diffusion coefficient is assumed to be a function of depth, and a one-dimensional contaminant diffusion model is proposed. The analytical solution satisfying all relevant conditions is derived by using orthogonal expansion method. According to the proposed solution, contaminant transport is analyzed and the effects of the related parameters are discussed. The method is relatively simple to be applied and can be used for evaluating experimental results, and for verifying more complex numerical models.

2 MATHEMATICAL MODEL

The major assumptions for the model are as follows: (1) contaminant diffusion model is one-dimensional; (2) the diffusion coefficient is a linear function of depth; (3) the retardation factor is constant; (4) adsorption is the linear type.

The governing equation for one-dimensional contaminant diffusion problem can be described as:

$$R \frac{\partial C(z,t)}{\partial t} = \frac{\partial}{\partial z} \left[ D(z) \frac{\partial C(z,t)}{\partial z} \right]$$  \hspace{1cm} (1)

where $C(z,t)$ is the contaminant concentration [ML$^{-3}$]; $R$ is the retardation factor; $D(z)$ is the diffusion coefficient [L$^{2}$T$^{-1}$], and is assumed to be a function of depth, i.e. $D(z) = D_0(a + bz)$. Here $D_0$ is an initial diffusion coefficient [L$^{2}$T$^{-1}$], $a, b$ are the heterogeneity parameters.

According to Liu et al (1998), the boundary conditions for the problem considered can be expressed as follows:

$$z = 0: C(0,t) = C_0$$  \hspace{1cm} (2)

$$z = H: C(H,t) = 0$$  \hspace{1cm} (3)

where $H$ is the thickness of the soil medium.

$$t = 0: C(z,0) = 0$$  \hspace{1cm} (4)

3 ANALYTICAL SOLUTION

According to the superposition principle, to convert the inhomogeneous boundary condition into a homogeneous one, the solution can be expressed as:

$$C(z,t) = u(z)C_0 + \theta(z,t)$$  \hspace{1cm} (5)

where the solutions of $u(z)$ and $\theta(z,t)$ are solved as follows.

3.1 Solution for $u(z)$

The governing equation for $u(z)$ is as follows:

$$\frac{d}{dz} \left[ D(z) \frac{d u(z)}{dz} \right] = 0$$  \hspace{1cm} (6)

The boundary conditions for this problem are:

$$z = 0: u(0) = 1$$  \hspace{1cm} (7)

$$z = H: u(H) = 0$$  \hspace{1cm} (8)

The solution to Eq.6 is:

$$u(z) = P + Q h(\frac{a}{b} + z)$$  \hspace{1cm} (9)

where $P$ and $Q$ can be obtained using the boundary conditions (Eqs.7,8).

3.2 Solution for $\theta(z,t)$

The governing equation for $\theta(z,t)$ can be written as follows:

$$R \frac{\partial \theta(z,t)}{\partial t} = \frac{\partial}{\partial z} \left[ D(z) \frac{\partial \theta(z,t)}{\partial z} \right]$$  \hspace{1cm} (10)

The boundary conditions for this problem are:

$$z = 0: \theta(0,t) = 0$$  \hspace{1cm} (11)

$$z = H: \theta(H,t) = 0$$  \hspace{1cm} (12)

The initial condition is:

$$t = 0: \theta(z,0) = -u(z)C_0$$  \hspace{1cm} (13)

According to the solution to homogeneous heat conduction problem, the solution of $\theta(z,t)$ can be expressed:

$$\theta(z,t) = \sum_{m=1}^{\infty} \xi_m e^{-\frac{\alpha_m^2}{4} t} \omega_m(z)$$  \hspace{1cm} (14)

With

$$\omega_m(z) = A_m J_0 \left( \frac{\beta_m}{\sqrt{\alpha}} \sqrt{a + bz} \right) + B_m Y_0 \left( \frac{\beta_m}{\sqrt{\alpha}} \sqrt{a + bz} \right)$$  \hspace{1cm} (15)

$$\alpha_m = \left( \frac{D_0}{R} \right) \left( \frac{a}{b} \right)^2$$  \hspace{1cm} (16)

$$\xi_m = -\frac{C_0 \int_0^H u(z) \omega_m(z) \, dz}{\int_0^H \omega_m^2(z) \, dz}$$  \hspace{1cm} (17)

where $J_0$ and $Y_0$ are zero-order Bessel functions of
the first kind and second kind. The parameters of $A_m$, $B_m$ and $\beta_m$ are determined by the boundary conditions.

Flux of contaminant can be obtained as follows:

$$J(z, t) = -nD_0 \frac{\partial C(z, t)}{\partial z} - nD_0C_0Qb$$

$$+ n \sqrt{D_0Ra + b} \sum_{m=1}^{\infty} \xi_m B_m e^{-\beta_m/\sqrt{a + bz}} [A_m J_m(\frac{\beta_m}{\sqrt{a + b}}) + B_m Y_m(\frac{\beta_m}{\sqrt{a + b}})]$$

(18)

where $J_i$ and $Y_i$ are first order Bessel functions of the first kind and second kind.

**4 ANALYSIS RESULTS AND DISCUSSION**

On the basis of the obtained analytical solution, the corresponding program is compiled and the contaminant transport in soil medium is illustrated. The values of relevant parameters are shown in Table 1.

| Parameter | Value |
|-----------|-------|
| $n$       | 0.3   |
| $D_0$     | $6.5 \times 10^{-11}$ |
| $R$       | 4.0   |
| $H$       | 1.0   |

Table 1 Property parameters of soil medium

Fig.1 shows the change of contaminant concentration with depth for different time. Here we set $a = 1$, $b = 15$. As shown in Fig. 1, the concentration of contaminant varies widely at different time. Fig.2 shows the variation of concentration with time for different depths. From the figure, we can see that the contaminant concentration increases with time at the beginning of a period of time, and reaches steady-state at around 100 years. In addition, the contaminant concentration decreases quickly with depth.

The effects of the initial diffusion coefficient and heterogeneity parameter on contaminant flux at the bottom are shown in Fig. 3 and Fig. 4. As shown in figures, the bottom contaminant flux has a great difference under different conditions. With the relevant parameters increasing, the contaminant flux also increases. The parameters not only affect the required time for reaching steady-state, but also have an impact on the stable value.
5 CONCLUSIONS

This paper presents an analytical solution for one-dimensional contaminant diffusion with distance-dependent diffusion coefficient. The analytical solution is obtained by using the orthogonal expansion method and the program is written through MATLAB.

Through the parameters study, it is found that the contaminant concentration is drastically reduced with the increase of depth, and the relevant parameters have an important impact on the calculation results. The contaminant concentration increases as the initial diffusion coefficient increases, and the initial diffusion coefficient only affect the time for contaminant concentration reaching steady-state. The required time of reaching steady-state is shorter and the contaminant concentration value of steady-state is smaller when the heterogeneity parameter is larger. So an accurate value of the diffusion coefficient is important to improve the prediction accuracy. The proposed model is established on the basis of linear adsorption, therefore it is necessary to make further research for considering non-linear adsorption and decay.

ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (Grant No.41372264), Zhejiang Provincial Natural Science Foundation of China (Grant No.LY13E080013), and Zhejiang Provincial Governmental Public Industry Research Special Funds for Projects (Grant No. 2014C33015 & 2015C333220).

REFERENCES

1) Benson C H, Daniel D E, Boutwell G P. (1999): Field performance of compacted clay liners. Journal of Geotechnical and Geoenvironmental Engineering, 125(5), 390-403.
2) Berger W, Kalbe U, Goebbels J. (2002): Fabric studies on contaminated minerals layers in composite liners. Applied Clay Science, 21(1-2),89-98.
3) Bezza A, Ghomari F. (2009): Nondestructive test to track pollutant transport into landfill liners. Environmental Geology, 57(2),285-290.
4) Chen J S, Ni C F, Liang C P, et al. (2008): Analytical power series solution for contaminant transport with hyperbolic asymptotic distance-dependent dispersivity. Journal of Hydrology, 362(1-2),142-149.
5) Chen Y G, Ye W M, Xie Z J, et al. (2012): Remediation of saturated Shanghai sandy silt contaminated with p-xylene using air sparging. Natural Hazards, 62(3),1005-1020.
6) Chen Y M, Xie H J, Ke H, et al. (2006): Analytical solution of contaminant diffusion through multi-layered soils. Chinese Journal of Geotechnical Engineering,28(4),521-524.(in Chinese)
7) Edil T B. (2003): A review of aqueous-phase VOC transport in modern landfill liners. Waste Management,23 (7),561-571.
8) Frempong E M, Yanful E K. (2008): Interactions between three tropical soils and municipal solid waste landfill leachate. Journal of Geotechnical and Geoenvironmental Engineering, 134(3),379-396.
9) Gordon M E, Huebner P M, Mitchell G R. (1990): Regulation, Construction and Performance of Clay-Lined Landfills in Wisconsin. Waste Contaminant Systems Geotechnical Special Publication, 26,14-27.
10) Guan C, Xie H J, Chen Y M, et al.(2012): Analytical solution for one dimensional contaminant diffusion through unsaturated soils beneath landfills. Journal of Civil, Architectural & Environmental Engineering, 34,93-98.(in Chinese)
11) Kalbe U, Muller W, Berger W, et al. (2002): Transport of organic contaminants within composite liner systems. Applied Clay Science, 21(1-2),67-76.
12) Kim J Y, Edil T B, Park J K. (2003): Volatile organic compound (VOC) transport through compacted clay. Journal of Geotechnical and Geoenvironmental Engineering,127(2),126-134.
13) Li Y C, Cleall P J.(2010): Analytical solutions for contaminant diffusion in double-layered porous media. Journal of Geotechnical and Geoenvironmental, 136(11), 1542-1554.
14) Liu C X, Ball W P. (1998): Analytical modeling of diffusion-limited contamination and decontamination in two-layer porous medium. Advances in Water Resources, 21(4),297-313.
15) Pérez G J S, Skaggs T H. (2010): Analytical solution for one-dimensional advection-dispersion transport equation with distance-dependent coefficients[J].Journal of Hydrology, 390(1-2),57-65.
16) Rowe R K, Nadarajah P. (1997): An analytical method for predicting the velocity field beneath landfills [J]. Canadian Geotechnical Journal, 34,264-282.
17) Shackelford C D, Lee J M. (2005): Analyzing diffusion by analogy with consolidation. Journal of Geotechnical and Geoenvironmental, 131(11),1345-1359.
18) Singh P. (2011): One dimensional solute transport originating from a exponentially decay type point source along unsteady flow through heterogeneous medium Journal of Water Resource and Protection, 3(8), 590-597.
19) Toupiol C, Willingham T W, Valocchi A J, et al. (2002): Long-term tritium transport through field-scale compacted soil liner. Journal of Geotechnical and Geoenvironmental Engineering, 128(8),640-650.
20) Wang C, Wang D G. (1996): Analytical solution of contaminant transport model with varying coefficients in groundwater system. Journal of Hydrodynamics, 11(4),475-484.(in Chinese)
21) Willingham T W, Werth C J, Valocchi A J, et al.( 2004): Evaluation of multidimensional solute transport through field-scale compacted soil liner. Journal of Geotechnical and Geoenvironmental Engineering, 130(9),887-895.
22) Xie H J, Chen Y M, Lou Z H. (2010): An analytical solution to contaminant transport through composite liners with geomembrane defects. Science China Technological Science-, 53(5),1424-1433.
23) You K H, Zhan H B. (2013): New solutions for solute transport in a finite column with distance-dependent dispersivities and time-dependent solute sources. Journal of Hydrology, 487,87-97.