The FUPG Finite Element Model of Contaminant Transportation in Soil with Nonlinear Sorption

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Summary The mathematical model of contaminant transportation with nonlinear equilibrium sorption of soil on the pollutant contamination in pore fluid was developed. The finite element model of the governing equations was developed with the Full Upwind Petrov-Galerkin method (FUPG). Numerical simulations were carried out with the developed program. The numerical results show the stability and the ability of the program to analysis the contaminant transportation of nonlinear equilibrium sorption in clay.

1 Introduction

Transportation of contaminants in the soil is a complex convection-diffusion-geochemical reactions [1-2] process. The application of traditional Galerkin method to solve the convection-diffusion problem in soil will lead to unstable solutions and numerical oscillations. These oscillations have amplitude with the increasing convective character of the problem.
A variety of methods to avoid numerical oscillation have been proposed. Brooks and Hughes proposed Streamline Upwind Petrov-Galerkin Method (SUPG) [3] which has space upwind weighting functions to avoid numerical oscillation. The Full Upwind Petrov-Galerkin Method (FUPG) proposed by Yu [4] has weighting functions which contain time and spatial upwind term. Radu [5] developed the Full Upwind Petrov-Galerkin Method, Li and Wu [6] developed the characteristic finite element model to solve the convection-diffusion equation of soil. In these models the linear adsorption models are selected. However, experiments [7-8] showed that the adsorption on metal ions and fearing water organic matter of soil are always nonlinear.
In the present paper, the mathematical model of contaminant migration in porous medium is developed basing on the migration mechanism of pollutants in porous medium and the conservation of mass. The finite element model of the governing equations is deduced based on the Full Upwind Petrov-Galerkin Method (FUPG), and the program of the model was developed.

2 Mathematical Model

Convection, molecular diffusion and mechanical dispersion are the main factors of contaminant transportation in soil. Adsorption, degradation and immobile water will influence the distribution of contaminants and delay the migration [6] . Experiments showed that soil has nonlinear adsorption effect on metal ions and fearing water organic matter. In the present paper the Langmuir isotherm adsorption is adopted to describe sorption on the solid to pollution:

$$F = \frac{K_1 K_2 c_m}{1 + K_1 c_m} \tag{1}$$

where: K_1 is the adsorption strength. K_2 is the adsorption capacity, c_m is concentration in mobile water.
Considering the basic pollutants transport phenomena, we can establish the mass conservation equations of pollutants in mobile water and solid skeleton of soil with nonlinear sorption considered:

$$\frac{\partial}{\partial t}\left(\theta_s \rho_s \frac{K_1 K_2 c_m}{1 + K_1 c_m}\right) = f_m^s \tag{2}$$

$$R_{dm}\frac{\partial c_m}{\partial t} + \nabla \bullet v_w c_m + v_w \nabla c_m - \nabla \bullet \left(\mathbf{D}_h \nabla c_m\right) = 0 \tag{3}$$

where: θ_s, θ_m are volume proportion of solid and mobile water. ρ_s are density of solid and mobile water. f_m^s is mass of pollutant going to the solid. And:

$$R_{dm} = 1 + \rho_s \frac{\theta_s}{\theta_m}\frac{K_1 K_2}{(1 + K_1 c_m)^2} \tag{4}$$

The weak form of the governing equation is received with FUPG method:

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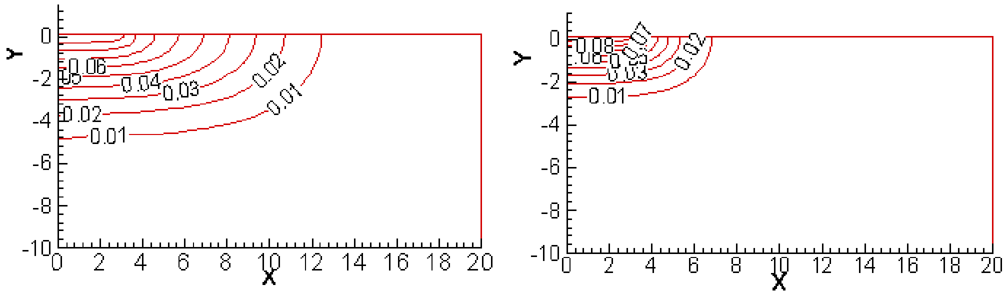
$$\Pi_{ej} = \int_{\Delta t}\int_{V_e}\left[R_{dm}\frac{\partial c_m}{\partial t} + \nabla \bullet v_w c_m + v_w \nabla c_m - \nabla \bullet \left(\mathbf{D}_h \nabla c_m\right)\right] W_j\left(x,t\right) dVdt \tag{5}$$

The weight functions are proposed by Yu C.C and Heinrich J.C [4] :

$$W_j\left(x,t\right) = N_j^x\left(x\right)W^t\left(t\right) + \Delta W_{j1}^x\left(x\right)W^t\left(t\right) + \Delta W_{j2}^x\left(x\right)\frac{\partial W^t\left(t\right)}{\partial t} \tag{6}$$

4 Numerical examples

There is clayey soil body which is 10m length and 20m wide. There is a constant horizontal velocity field with vwx=6.3×10^{-8}m/s in the soil, Dm=3.0×10^{-8}m^2/s. There is a constant concentration on the left top boundary of 2.8m width. To study the effect of nonlinear sorption on the transportation of contaminant in pore water of soil, different adsorption parameters are selected. There are two cases for the calculation: ①K1=0.11 and K2=1; ②K1=0.11 and K2=12.87 [9] . The concentration distribution of 1800d was exhibited in Fig. 1. The numerical results show that the solution is stable. With K2 increasing, the migration of contaminant is delayed because of the adsorption on the contaminant is reinforced, which suggest that K2 is the controls parameter of pollution migration in clayey soil because of sorption.



(a) K1=0.11 and K2=1 (b) K1=0.11 and K2=12.87

Fig. 1 The concentration distribution of 1800d

6 Conclusions

Considering the basic pollutants transport phenomena, we can establish the mass conservation equations of pollutants in mobile water and solid skeleton of soil with nonlinear sorption considered. The finite element mode is developed with FUGP method. The numerical simulation with the program is carried out, and the numerical results showed the stability and the capability of the current model to simulate the convection-diffusion transportation of contaminant in soil.

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REFERENCES

[1] Zhang J.L., Luan M.T.,Yang Q., Numerical analysis of landfill leachate migration processes considering nonlinear equilibrium sorption behaviour of CCL [J]. Chinese Journal of Computational Mechanics,25(2):162-168, 2008.

[2] Harmas H., Zzhnder A. J. B. Bioavailability of asorbed-chlorodibenzofuran[J]. Applied Environment Microbiology,61(1):27-33, 1995.

[3] Brooks A N, Hughes T J R. Streamline upwind Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible navier-stokes equations [J]. Comput Methods in Applied Mechanics and Engineering,32:199-259, 1982.

[4] Yu C.C., Heinrich J.C., Petrov-Galerkin methods for multidimensional time dependent convective-diffusion equations[J]. International Journal for Numerical Methods in Engineering,24:2201-2215, 1987.

[5] Radu J.P., Biver P., CHARLIER R., et al. 2D and 3D finite element modeling of miscible pollutant transport in g roundwater. Below the unsaturated zone. Int conf. on hydrodynamics Wuxi China. 1994.

[6] Li X.K., Wu W.H., Characteristic Galerkin Method for convection-diffusion equations and implicit algorithm using precise integration. Acta Mechanica Sinica,15(4): 371-382, 1999.

[7] Claudia F., Werner S., Stefan B. H., et al. Nonlinear sorption and non-equilibrium solute transport in aggregated porous media: experiments, process identification and modeling[J]. J. Contam Hydrol,31:373-407, 1998.

[8] Malcolm S. F., Paul F. P., A two-region non-equilibrium model for solute transport in solution conduits in Karstic aquifers[J]. J. Contam Hydrol, 44: 329-351, 2000.

[9] Lu J.S., Wu Y.Q. Mu C.W., et al, Modelling trichloroethylene transport in porous media based on advection-diffusion equation coupled with nonlinear adsorption. Ecology and Environment，17(1)：28-34, 2008