Predicting the Transport of Chlorinated Organics in Groundwater with Mathematical Methods

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Abstract. A previous study showed a developed mathematical model could describe the transport of perchloroethylene (PCE) in the simulating column. This study tried to use the model to predict the transport of pollutant in low organic carbon content aquifer. The results told that the concentration variation characteristics in the flow direction in continuous input and finite duration input mode of pollutants. More useful information can be obtained through changing some parameters values. The application of mathematical model in prediction has been helpful in the prevention and remediation of groundwater contamination.

Introduction

Groundwater contamination has been reported more and more frequently in recent years [1]. It is essential to know the transport process and the fate of contaminants for groundwater contamination prevention. For accidental pollution, the accurate prediction of the fate of pollutants is very useful for the decision of the management and remediation strategy. Once solutes enter aquifer, they will usually undergo dispersion, advection, sorption, chemical reaction, biodegradation and so on [2]. The transport of hazardous organic contaminants in groundwater is markedly affected by the extent of their sorption which depends largely on the organic content of media. For the porous media materials with low organic carbon content (f_{oc}), the sorption isotherm is often not linear [3]. It suggests that the classical advection-dispersion equation may be improper to describe the transport of the organics in low f_{oc} aquifer media.

The previous study demonstrated that the sorption isotherms of perchloroethylene (PCE) in low f_{oc} sandy aquifer fitted the amended dual-mode (DMM) [4], as a subsequent work, the mathematical equation as an transport model has been developed to describe the transport of solute in low f_{oc} aquifer; and then the transport model would be tried to predict the transport of PCE in low f_{oc} aquifer, including the concentration variation characteristics of solute along the time at different distance from the pollution source, especially in three kinds of aquifer materials.

Materials and Methods

This study selected three sandy media as the representative of low f_{oc} aquifer materials. Three sandy media were natural coastal sediments with simple pretreatment [3], the physiochemical properties are listed in Table 1.

Table 1 Properties and parameters value of media A, B and C

media	dry bulk density ρ [g/cm^3]	particle diameter [mm]	porosity [θ]	organic carbon f_{oc}[%]	average pore diameter [nm]
A	1.32	0.125~0.25	0.45	0.090	8.848
B	1.40	0.063~0.125	0.44	0.086	8.857
C	1.68	<0.063	0.42	0.080	9.188

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Results and Discussions

Transport mathematical model. Mathematical model were deduced from the classical advection-dispersion equation, during several days, the transformation of chlorinated organics can be ignored because of its scarce biodegradation. Therefore the transport of PCE in one-dimensional steady-state flow in a homogeneous, isotropic porous media can be described by

$$\left[1+\frac{\rho}{\theta}K_d+\frac{\rho}{\theta}q_0 b\frac{1}{(1+bC)^2}\right]\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-v\frac{\partial C}{\partial x}\quad(1)$$

Where C is the concentration of solute in liquid phase; C_0 is the initial concentration of solute injection; t is the time; D is the hydrodynamic dispersion coefficient; v is the average pore velocity; ρ is the bulk density of porous media; θ is the porosity of porous media; x is the distance in water flow direction; K_d, q_0, b are parameters in DMM sorption model [3].

For continuous input, the initial and boundary conditions are given as

$$\begin{cases} C(x,t=0)=0 \\ C(x=0,t>0)=C0 \\ C(x\to\infty,t)=0 \end{cases}\quad(2)$$

For finite duration input, the initial and boundary conditions are given as

$$\begin{cases} C(x,t=0)=0 \\ C(x=0,0<t<t_i)=C_0 \\ C(x=0,t>t_i)=0 \\ C(x\to\infty,t)=0 \end{cases}\quad(3)$$

Prediction the transport of pollutant in continuous input mode. The mathematical model (Eq.1 and Eq.2) was used to predict the transport of PCE in three aquifers similar to media A, B and C mentioned above. Supposed the accidental pollution of PCE has the initial concentration less than 16.300 mg/L (the concentration limit was selected just in order to utilize directly the first hand sorption parameters obtained from batch tests), the concentration characteristics of PCE at 100cm site far from the pollution source in the flow direction are shown in Fig. 1, also supposed that the aquifer materials was similar to media A. The parameters values used in transport model are listed in Table 2. It can be seen from Fig.1 that the higher the source concentration is, the more quickly the pollution plume reached, and the shorter the breakthrough time is. For example, the breakthrough time costs only 0.4 day if the source concentration is 16.3 mg/L, while it costs 0.9 day and 1.1 day if the source concentration is 6.52 mg/L and 1.63 mg/L respectively. It suggested that the lower the source concentration was, the stronger the retardation was. Fig. 2 shows the concentration characteristics at 200cm site far from the source in the flow direction in the aquifer similar to media B, while Fig. 3 is at 300cm site far from source in aquifer similar to media C. The parameters values are also listed in Table 2. The similar breakthrough characteristics to media A can be seen in media B and C from Fig. 2 and Fig.3. It can be suggested that the breakthrough time was affected largely by the pollution source concentration.

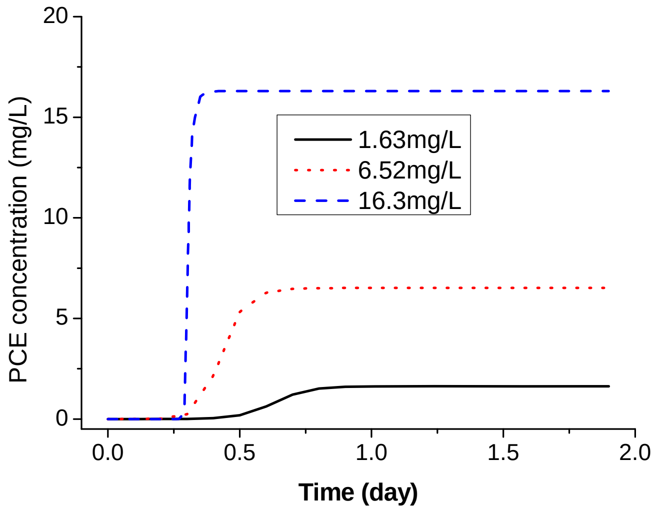

Fig. 1 Concentration characteristics of PCE in aquifer similar to media A at 100cm site far from the source in the flow direction in continuous input mode (three line represents the different initial source concentration respectively)

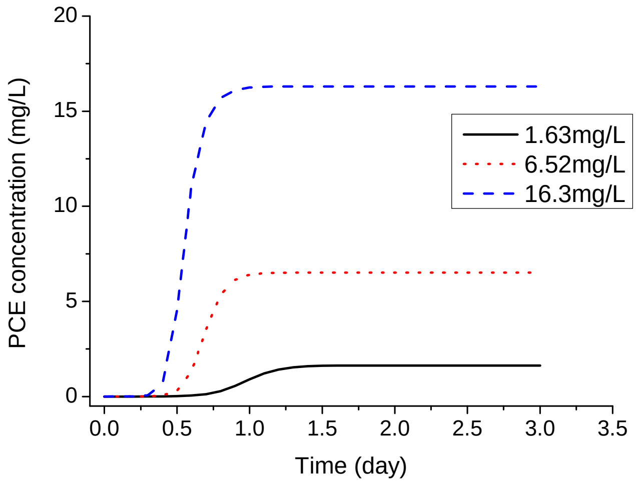

Fig. 2 Concentration characteristics of PCE in aquifer similar to media B at 200cm site far from the source in the flow direction in continuous input mode (three line represents the different initial source concentration respectively)

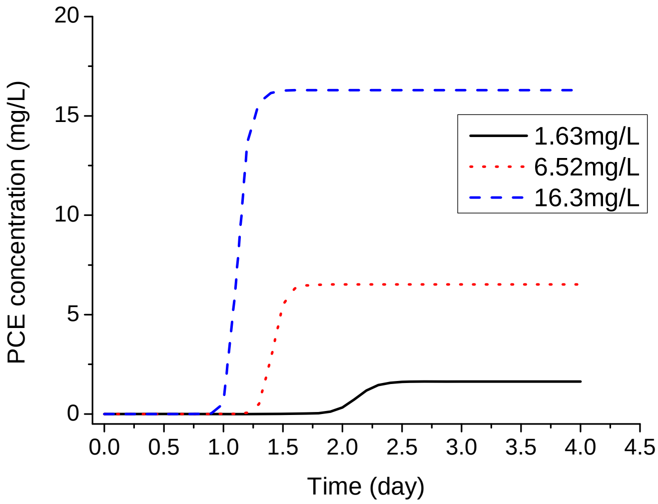

Fig. 3 Concentration characteristics of PCE in aquifer similar to media C at 300cm site far from the source in the flow direction in continuous input mode (three line represents the different initial source concentration respectively)

Table 2 Parameters value of transport model of PCE in aquifer in continuous input mode

aquifer properties	Media A	Media B	Media C
hydrodynamic dispersion coefficient (D)[cm^2/min]	0.31	0.30	0.27
average pore velocity (v)[cm/min]	0.52	0.50	0.45
distribution coefficient (K_d)[L/mg]	0.08	0.04	0.03
maximum adsorption capacity (q_0) [mg/kg]	2.18	2.68	2.42
sorption constant (b)[L/kg]	1.31	0.47	0.81
porosity[θ]	0.45	0.44	0.42
bulk density (ρ)[g/cm^3]	1.32	1.40	1.68
distance (x)[cm]	100	200	300
	1.63	1.63	1.63
initial concentration (C_0)[mg/L]	6.52	6.52	6.52
	16.3	16.3	16.3

Prediction the transport of pollutant in finite duration input mode. The mathematical model (Eq.1 and Eq.3) was used to predict the transport of PCE in finite duration input mode in three aquifers similar to media A, B and C mentioned above. The parameters values used in transport model are listed in Table 3. Fig. 4 shows the concentration characteristics variation of PCE in aquifer similar to media A at 100, 200, 300 cm sites in the flow direction in 1 day finite duration input mode. The source concentration was 16.3 mg/L, under the condition of 1 day finite duration input, at 100cm site far from the source in the flow direction, the concentration of PCE ascended rapidly in several hours, the peak value of PCE reached to 16.3 mg/L and remained within several hours, and then became to decline till to zero after about 5 days. At 300cm site far from the source, the concentration variation of PCE has a wave pattern similar to that of 100cm site with a 14.5 mg/L peak value. It was suggested that some of solute had been adsorbed to aquifer materials or retarded in aquifer. It implied that in finite duration input mode, the pollution plume would not reach to those sites enough far away for ever, and natural aquifer had the capacity for some pollutants. It can also be seen from Fig.4 that at different sites, concentration variation in ascending stage was rapider than that in descending stage; it was the explanation of the adsorption retardation in the transport of solute.

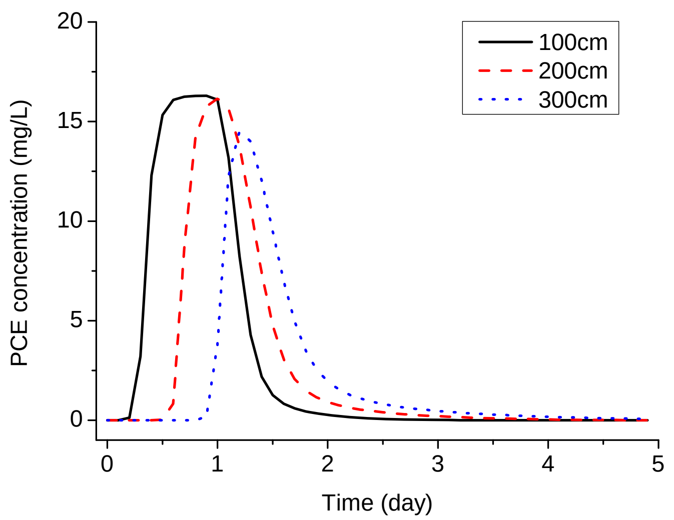

Fig. 4 Concentration variation characteristics of PCE in aquifer similar to media A at different sites in the flow direction in 1 day finite duration input mode (three lines represent three sites far from pollution source respectively)

Table 3 Parameters values of transport model of PCE in aquifer in finite duration input mode

aquifer properties	Media A	Media B	Media C
hydrodynamic dispersion coefficient (D)[cm^2/min]	0.31	0.30	0.27
average pore velocity (v)[cm/min]	0.52	0.50	0.45
distribution coefficient (K_d)[L/mg]	0.08	0.04	0.03
maximum adsorption capacity (q_0) [mg/kg]	2.18	2.68	2.42
sorption constant (b)[L/kg]	1.31	0.47	0.81
porosity (θ)	0.45	0.44	0.42
bulk density (ρ)[g/cm^3]	1.32	1.40	1.68
initial concentration (C_0)[mg/L]	16.3	16.3	16.3
finite duration input [day]	1	2	3
	100	100	100
distance (x)[cm]	200	200	200
	300	300	300

Fig. 5 shows the concentration characteristics variation of PCE in aquifer similar to media B at 100, 200, 300 cm sites in the flow direction in 2 days finite duration input mode. Fig.6 shows that of media C in 3 days finite duration input mode. The parameters values used in transport model are also listed in Table 3. It can be seen that the concentration characteristics variations were similar to that in aquifer A, at any site in the flow direction, the concentration of PCE began to ascend rapidly, then reached to the peak value of 16.3 mg/L lasting some time, and then began to descend slowly, till to zero after several days. It could be also seen from Fig.5 and Fig.6 that the longer the input duration was, the longer time the peak value remained. It suggested that the adsorption capacity at that site had been saturated.

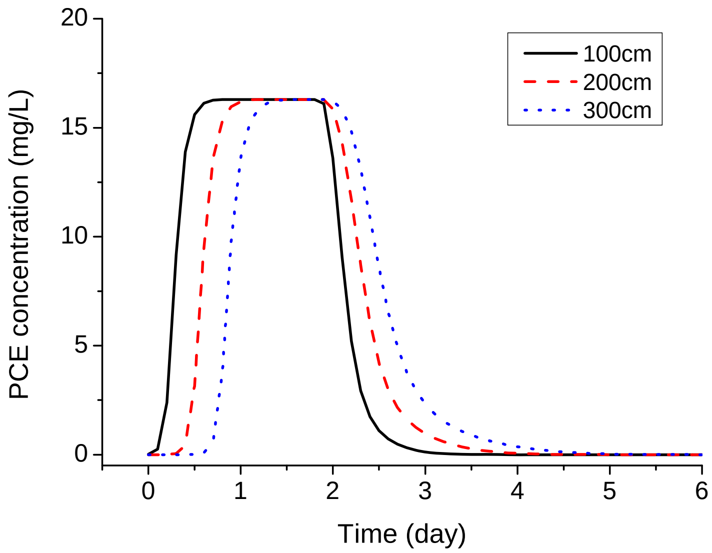

Fig. 5 Concentration characteristics variation of PCE in aquifer similar to media B at different sites in the flow direction in 2 days finite duration input mode (three lines represent three sites far from pollution source respectively)

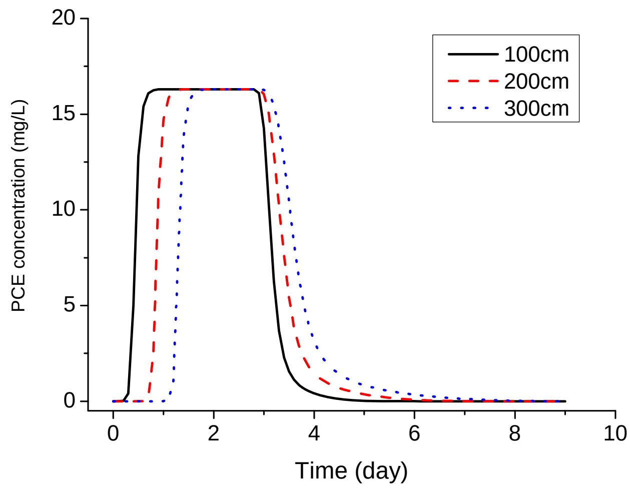

Fig. 6 Concentration characteristics variation of PCE in aquifer similar to media C at different sites in the flow direction in 3 days finite duration input mode (three lines represent three sites far from pollution source respectively)

Conclusion

The prediction in this study suggests that the mathematical transport model can be used widely in a convenient way. After the amendment based on the investigation practice, the mathematical model can easily tell the transport characteristics of pollutants through changing any parameter value such as dispersion coefficient, pore velocity, initial concentration or input mode. Mathematical methods are very helpful in the prevention and remediation of groundwater pollution.

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