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MODELING TRANSPORT AND FATE OF CHLORINATED HYDROCARBONS GOVERNED BY BIOTIC TRANSFORMATION IN POROUS MEDIA

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Abstract—A macroscopic partitioning model governed by microbial transformation was developed to elucidate the transport and fate of chlorinated hydrocarbons and microorganisms in porous media. Carbon tetrachloride (CT) and 1,1,1-trichloroethane (TCA) were selected as the target compounds. A laboratory column experiment was also conducted to validate the accuracy of the model. Results obtained from the TOC concentration and microbial activities in effluent and pore water demonstrate that the steady state of the microbial growth was reached after an incubation period of 40 days. Microorganisms tended to accumulate in the first 20 cm of the column and consumed auxiliary substrate rapidly to sustain the dechlorinating capabilities. Significant degradation of CT with the concomitant increase of chloroform, the daughter product of CT via dechlorination, was also demonstrated after 57 days. TCA is more recalcitrant than CT. Removal of 42% of the original TCA input was demonstrated in 121 days. No 1,1-dichloroethane was detected. Model simulation results indicate that the predicted concentrations are all in the range close to the experimental data. A good correlation between the simulated and measured values demonstrates that the partitioning model can describe the transport and fate of chlorinated hydrocarbons and microorganisms in the contaminated groundwaters. The distribution coefficient between free-living and attached bacteria plays a prominent role in controlling the distribution pattern of microorganisms and the fate of chlorinated hydrocarbons. In addition, the interaction between the supplemental substrate and the active microorganisms significantly influences the dechlorination of chlorinated hydrocarbons. The valid and accurate transport model provides the basis for the accurate prediction of the transport and fate of chlorinated hydrocarbons as well as the proper selection of a remedial approach to eliminate contaminants in soil environments.

Key words—carbon tetrachloride, 1,1,1-trichloroethane, macroscopic partitioning model, biotransformation, free-living bacteria, attached bacteria, modeling

INTRODUCTION

Groundwater and soil contamination by chlorinated hydrocarbons has recently become of increasing concern (McNab and Narasimhan, 1994). Annual consumption of chlorinated hydrocarbons in Taiwan, primarily used as degreasing agents and cleaning solvents, is estimated to be around 3.6×10^5 t. In light of their widespread usage and improper disposal, these contaminates have migrated into the subsurface and pose a health threat owing to their suspected carcinogenicities and mutagenicities. Previous studies have demonstrated *in situ* bioremediation to be a cost-effective remedial approach (Doong and Wu, 1995). However, managing remedial action is often hindered by an inadequate understanding of the basic processes which transport hazardous materials into the environment. An urgent requirement has arisen to thoroughly understand the behavior of chlorinated hydrocarbons in the environments as well as successfully apply remedial techniques.

Biological transformation is widely recognized as a critical mechanism in the attenuation of xenobiotics (Ghiorse and Wilson, 1988; Sewell and Gibson, 1991). Under anoxic/anaerobic conditions, chlorinated hydrocarbon can be fortuitously biotransformed via reduction dechlorination to produce a series of lower chlorinated homologs. Research has demonstrated that microbial and substrate concentrations, electron acceptors and oxidation-reduction potential of the environment are the crucial environmental factors in determining the rate of

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dechlorination (Freedman and Gossett, 1988; Doong *et al.*, 1996). Moreover, previous work demonstrated that adding a low concentration of auxiliary would enhance the dechlorination efficiencies of chlorinated hydrocarbons under a reducing environment (Doong and Wu, 1995, 1996).

In soil environments, microorganisms can either attach to a soil surface to form biofilm or freely float in the pore water. Several studies have shown that these bacteria adhere primarily to the solid matrix (Harvey *et al.*, 1984; Federle *et al.*, 1986). Harvey *et al.* (1984) observed that microcolonies of between 10 and 100 bacteria are a common feature on the particle surface. However, Fontes *et al.* (1991) reported that significant numbers of bacteria can be removed through porous media, even when the percentage retained is extremely high. This finding gives an impetus to thoroughly understand the fate of microorganisms so as to more accurately predict the fate of chlorinated hydrocarbons in the subsurface environment.

Extensive literature has recently provided mathematical models describing the transport and fate of xenobiotics (Borden and Bedient, 1986; Baveye and Valocchi, 1989; MacQuarrie *et al.*, 1990; Zysset *et al.*, 1994). The dynamic behavior of microorganisms in porous media can generally be described by different conceptual models, i.e. the biofilm model, the microcolony model and the partitioning model, according to the manner in which bacteria grows in the surrounding environments. Among these models, the partitioning model is preferred in modeling the macroscopic transport behavior of xenobiotics under the premise that it does not make any unwarranted assumption concerning the spatial distribution of the biomass (Baveye and Valocchi, 1989; Zysset *et al.*, 1994). However, modeling transport of chlorinated hydrocarbons with microbial anaerobic dechlorination is less prevalent, and the microbial effects on the anaerobic dechlorination of chlorinated hydrocarbons still remain unclear.

In this study, simulating the biodegradation of chlorinated hydrocarbons and supplemental electron donor as well as the growth of microorganisms is of primary concern. A macroscopic partitioning model governed by microbial transformation was developed to describe the transport and fate of chlorinated hydrocarbons in porous media. Carbon tetrachloride (CT) and 1,1,1-trichloroethane (TCA) are selected as the target compounds. These compounds are promulgated as volatile organic contaminants under the Safe Drinking Water Act Amendments of the US Environmental Protection Agency, with the proposed maximum contaminant level in drinking water of 5 and 200 μg/liter for CT and TCA, respectively. The model is validated by a laboratory column experiment. Furthermore, the behavior of biomass is simulated as the basis for interpreting the fate of chlorinated hydrocarbons in a porous media.

THEORY AND BACKGROUND

The general governing equation describing the transport of a dilute solute in a saturated porous medium is as follows (Bear, 1979):

$$\frac{\partial C}{\partial t} = \mathrm{div}(D\cdot \mathrm{grad}C) - v\mathrm{grad}C - \frac{\rho(1-\theta)}{n_e}\frac{\partial S}{\partial t} + \left(\frac{\partial C}{\partial t}\right)_{\mathrm{rxn}} \quad (1)$$

where C is the mass concentration of the solute in the liquid phase (M/L^3), t is time (T), v is the average linear velocity (M/T), ρ is the density of the porous medium (M/L^3), S is the mass concentration of the solute adsorbed in the solid phase, θ is the water content, D is the hydrodynamic dispersion coefficient (L^2/T) and n_e is the effective porosity of the medium.

Under anaerobic condition, a supplemental substrate is required to initiate and sustain the dechlorinating capabilities of microorganisms (Freedman and Gossett, 1988; Doong and Wu, 1996). The growth of microorganisms and the removal of chlorinated hydrocarbons and auxiliary substrate can generally be quantified by Monod equation. Thus, the transport model undergoing advection, dispersion, linear sorption and biodegradation can be established by reducing equation (1) to one dimensional form

$$\frac{\partial C_h}{\partial t} = \frac{D_h}{R_{dh}}\frac{\partial^2 C_h}{\partial Z^2} - \frac{v}{R_{dh}}\frac{\partial C_h}{\partial Z} - \frac{k_h X_t C_h}{K_{sh} + C_h} \quad (2)$$

$$\frac{\partial C_p}{\partial t} = \frac{D_p}{R_{dp}}\frac{\partial^2 C_p}{\partial Z^2} - \frac{v}{R_{dp}}\frac{\partial C_p}{\partial Z} - \frac{k_p X_t C_p}{K_{sp} + C_p} \quad (3)$$

where subscript h denotes the chlorinated hydrocarbons, p denotes the auxiliary substrate, Z is the distance, X_t is the total biomass in the porous media, k is the maximum utilization rate of substrate, K_s is the half-saturation constant and R_d is the retardation factor of substrate as demonstrated by Freeze and Cherry (1979).

Appropriately simulating the transport of the microbial population requires developing an equilibrium distribution function capable of quantifying the ratio of the free-living bacterial concentration (X_s) to the attached biofilm density (X_f), k_x, i.e.

$$X_f = k_x X_s \quad (4)$$

Thus, the total biomass in the porous medium can be given by

$$X_t = (1-\theta)\alpha X_f + \theta X_s \quad (5)$$

where α is the surface area per unit volume of the porous medium. The variation of X_t in the porous

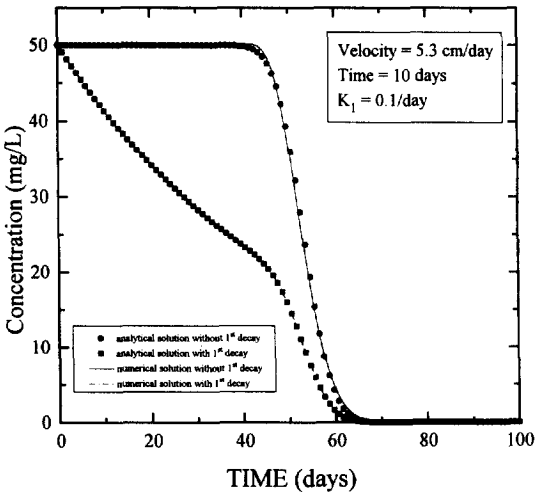

Fig. 1. Comparison of numerical solutions to the analytical solutions of the advection–dispersion equation with and without a first-order reaction term: k_1 is the first-order rate constant (day^{-1}), (●) represents the analytical solution without the first-order reaction term, (■) represents analytical solution with first-order decay term and the solid and dashed lines represent numerical solutions without and with the first-order reaction term, respectively.

medium can therefore be described via a mass balance equation:

$$\frac{\partial X_t}{\partial t} = \frac{D_x}{(1-\theta)\alpha k_x + \theta}\frac{\partial^2 X_t}{\partial Z^2} - \frac{v}{(1-\theta)\alpha k_x + \theta} \times \frac{\partial X_t}{\partial Z} + \mu_m X_t \frac{C_p}{K_s + C_p} - bX_t \quad (6)$$

where μ_m is the maximum growth rate, b is the decay rate. A situation is considered in which the concentration of chlorinated hydrocarbons (C_h) is significantly less than K_{sh}. Thus, the dechlorination reaction (equation 2) can be reduced to the second-order rate reaction:

$$\frac{\partial C_h}{\partial t} = \frac{D_h}{R_{dh}}\frac{\partial^2 C_h}{\partial Z^2} - \frac{v}{R_{dh}}\frac{\partial C_h}{\partial Z} - k_2 X_t C_h \quad (7)$$

Equations (3), (6) and (7) are solved by the implicit Crank–Nicolson finite difference method. Moreover, the numerical program is validated by verifying the model via the analytical solutions of the advection–dispersion equation with and without a first-order reaction term by assuming that $K_s \gg C_h$ and $X_t = 0$, respectively. Figure 1 compares the concentration profiles of the target compound obtained from numerical and analytical solutions of the developed model at 10 days. Table 1 summarizes the initial and boundary conditions and the input transport parameters used for comparison. The agreement between the two solutions is seen to be excellent, verifying that the developed model can simulate the processes of advection, dispersion, retardation and biological reaction.

MATERIALS AND METHODS

Culture and media

Anaerobic mix-culture consortia was obtained from the anaerobic biosolid of the Taiwan Sugar Corporation wastewater treatment facility (Hsinchu, Taiwan). It was then incubated at 35°C in a 2-liter glass flask with a magnetic stirrer under anaerobic condition. Supplementing the auxiliary substrate solution was curtailed for 2–3 days prior to the beginning of each experiment to exhaust the residual carbon sources in the anaerobic culture.

Phosphate-buffered mineral media used to incubate microcosms contained the following (per liter): 3.0 g of $Na_2HPO_4 \cdot 12H_2O$, 1.3 g of KH_2PO_4, 0.2 g of $MgCl_2 \cdot 6H_2O$, 0.9 g of NH_4Cl, 10 ml of trace metal solution and 3 ml of vitamin solution. The trace metal solution consisted of the following (per liter): 530 mg of $CaCl_2 \cdot 2H_2O$, 200 mg of $FeCl_2 \cdot 4H_2O$, 20 mg of $MnCl_2 \cdot 4H_2O$, 40 mg of $CuCl_2 \cdot 2H_2O$, 20 mg of $ZnCl_2$, 3 mg of H_3BO_3, 4 mg of $CoCl_2 \cdot 6H_2O$ and 4 mg of $Na_2MoO_4 \cdot 2H_2O$. The vitamin solution contained the following (per liter): 2 mg of biotin, 2 mg of folic acid, 5 mg of riboflavin, 10 mg of pyridoxine hydrochloride, 5 mg of thiamin, 5 mg of nicotinic acid, 5 mg of thioctic acid and 0.1 mg of vitamin B_{12}. Sodium sulfide ($Na_2S \cdot 9H_2O$), acting as a reducing agent, was introduced to give a concentration of 500 mg/liter. The initial pH of medium was 7.1 ± 0.2.

Column experiments

Two laboratory-scale, porous medium columns with 2-cm internal diameter by 100-cm long filled with 0.5-mm glass beads and seeded with mixed bacterial cultures under anaerobic condition were used to determine the behaviors of chlorinated hydrocarbons, supplemental substrate and biomass in porous media. Sampling ports were placed every 10 cm and capped with serum caps to prevent the

Table 1. The initial and boundary conditions and the input transport parameters used for comparison of the concentration profiles between numerical and analytical solutions

Initial conditions			
$C_p(0, Z) = 0$	at $Z > 0$		
$C_h(0, Z) = 0$	at $Z > 0$		
$X_t(0, Z) = X_{to}$	at $Z > 0$		
Boundary conditions			
$C_p(t, 0) = C_{po}$	at $t > 0$;	$dC_p/dZ = 0$	at $Z = L$, $t > 0$
$C_h(t, 0) = C_{ho}$	at $t > 0$;	$dC_h/dZ = 0$	at $Z = L$, $t > 0$
$X_t(t, 0) = 0$	at $t > 0$;	$dX_t/dZ = 0$	at $Z = L$, $t > 0$
Parameters			
θ	0.39 cm^3/cm^3	ρ_b	1.47 g/cm^3
v	5.3 cm/day	α	73.2 cm^2/cm^3
C_{po}	50.0 μg-C/ml	C_{ho}	50.0 μg/ml
X_{to}	50.0 μg-C/ml	L	100 cm
k_x	0.02 cm	k_2	0.002 (liters/mg)/day

volatilization loss of chlorinated hydrocarbons. Glass beads were used as the support media for microorganisms to minimize the sorptive effect.

Anaerobic mineral medium containing nutrients, supplemental substrate (glucose) and chlorinated hydrocarbons were injected into the column by a syringe pump with the superficial flow velocity of 12.2 cm/day. The final input concentrations of glucose and chlorinated hydrocarbons were 50 mg/liter and 100 μg/liter, respectively. Samples for chlorinated hydrocarbons, total organic carbon (TOC) and microbial activity determination were taken from the sampling ports, effluent stream and feed reservoir periodically to monitor the fate of chlorinated hydrocarbons and microorganisms.

Analytical methods

Concentrations of chlorinated compounds in the effluent and pore water were monitored by a Hewlett-Packard 5890A gas chromatography (Avondale, PA, USA) equipped with an electron capture detector (ECD) and a 3392A integrator. A 30-m DB-624 fused-silica megabore capillary column (0.53 mm i.d., 3.0 μm film thickness, J & W Scientific, Folsom, CA, USA) was used for separating the chlorinated compounds. The column temperature was maintained at 35°C for 1 min, then programmed to 50°C at the rate of 2°C/min and heated to 150°C at the rate of 8°C/min with a carrier gas (N_2) flow rate of 5.6 ml/min (linear velocity of 42.3 cm/s).

Oxidation-reduction potential (ORP) and pH values were determined with an Orion EA 920 expandable ion analyzer (Orion Research, Boston, MA, USA) by using an Orion gel-filled combination pH electrode for pH measurement and an Orion model 97-78-00 Pt redox electrode for ORP measurement. The ORP values in the experimental course ranged between −30 mV and −340 mV, which can be considered as a reducing environment. TOC concentration was obtained by a model 700 TOC analyzer (O. I. Corp., TX, USA) after filtering the liquid in a test bottle through a 0.2 μm cellulose nitrate membrane filter (47 mm, MFS, Dublin, CA, USA).

Enumeration of microbial activities in the solutions was determined in test bottles by an epifluorescence technique, the DAPI method (Coleman, 1980). An epifluorescence microscope equipped with a Nikon mercury lamp supply HB0-100W/2 (Nikon, Tokyo, Japan) was used to count the numbers of viable cells of each sample. Sample (10 ml) was fixed with 0.5 ml of filtered Formalin (37% formaldehyde) and was stained with 1 ml of DAPI solution at the concentration of 0.1 mg/ml (with a final concentration of 0.01 mg/ml).

RESULTS AND DISCUSSION

Column experiments

A laboratory column anaerobic experiment was conducted to determine whether the conventional transport equations adequately described the behaviors of chlorinated hydrocarbons and microorganisms in porous media as they undergo advection, dispersion and biodegradation. The concentrations of TOC in effluent and pore water demonstrate that the steady state was reached in the incubation period of 40 days. As illustrated in Fig. 2(A), greater than 90% of the input TOC were depleted and only a slight variation of TOC concentration of effluent was found. In addition, the TOC concentration of pore water was rapidly declined with distance near the beginning end of the column (Fig. 2B). Moreover, the

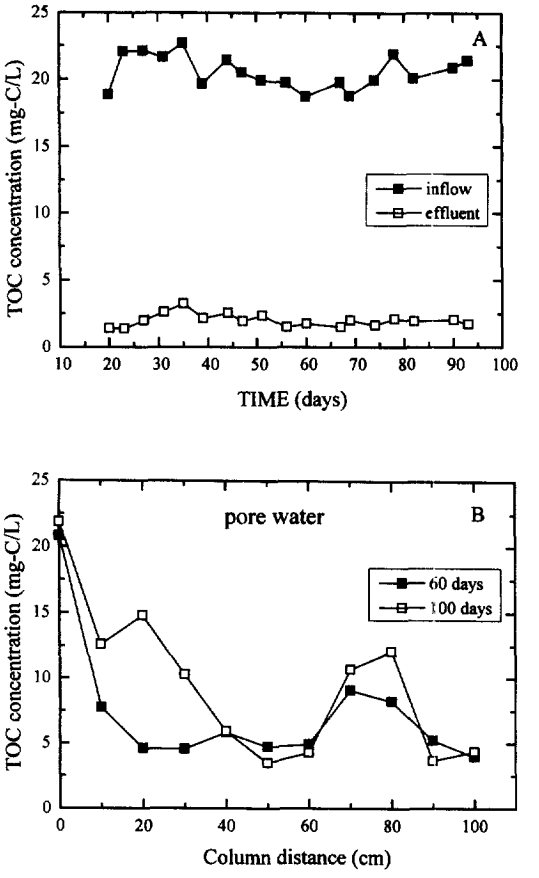

Fig. 2. The TOC concentration profiles of effluent and pore water in the laboratory column experiment.

microbial activity decreased from 1.4×10^5 cells/ml in the origin to 3×10^4 cells/ml at day 40 (Fig. 3) and then maintained nearly a constant value in 93 days. These results demonstrate that a large amount of the originally inoculated microorganisms were washed out. Nevertheless, some bacteria were retained by filtration and obtained energy for growth by consuming auxiliary substrate, subsequently accumulating a higher concentration of biomass in the top of column.

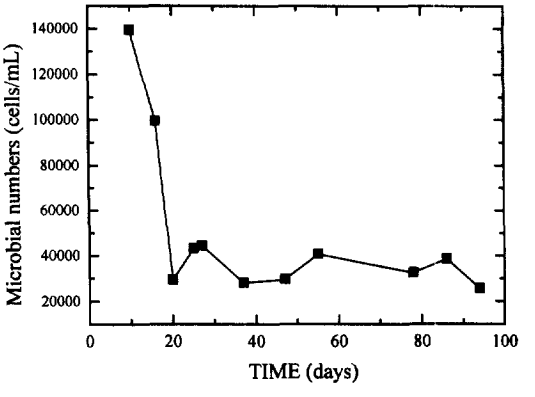

Fig. 3. Variation of the microbial density in effluent.

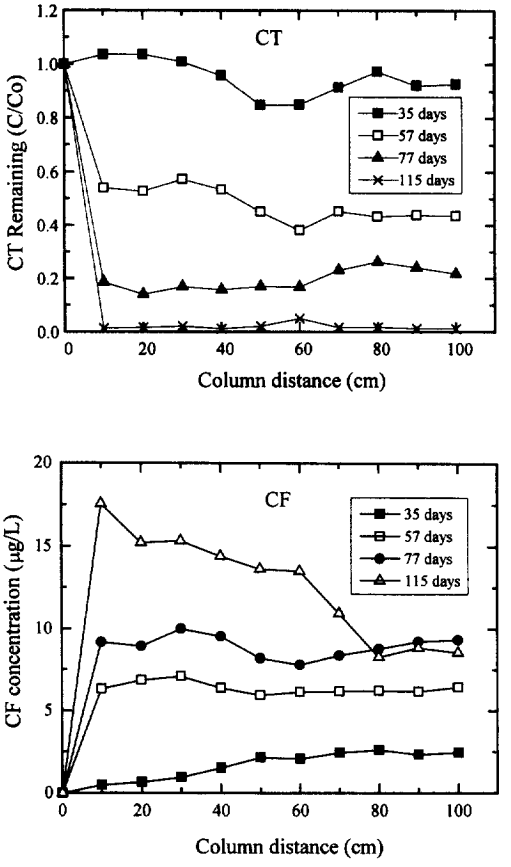

Fig. 4. The concentration profiles of CT and CF as a function of column distance. CF is the daughter product of CT via reductive dechlorination.

Figure 4 illustrates the concentration profiles of CT and chloroform (CF) along the column distance. No obvious degradation of CT occurred within 35 days, whereas a significant degradation was observed after 57 days. Near complete dechlorination of CT removal was exhibited in 121 days, occurring primarily in the first 10 cm of the column. In addition, CT was found to be degraded by reductive dechlorination to CF. However, only small amounts of CF, accounting for 6–17% of the CT lost, were observed. No formation of methylene chloride was detected, although CF decreased with time. These results indicate that the dechlorination of CT did not yield the stoichmetric amounts of the products. Other products such as radical coupling or water-soluble compounds may be formed in the test system (Criddle *et al.*, 1990; Matheson and Tratnyek, 1994).

TCA is a more recalcitrant compound than CT. As depicted in Fig. 5, TCA began to degrade after 77 days. Removal of 42% of the original TCA was achieved within 121 days. No 1,1-dichloroethane was detected. No significant difference of removal efficiency between 77 and 121 days was demonstrated. The active organisms likely had a limit capacity of TCA transformation. Galli and McCarty (1989) also reported that the TCA transformation activities of the nongrowing organisms decreased in the absence of a growth substrate when *Clostridium* sp. strain TCAIIB was used to transform high concentrations of TCA. In the present study, only 50 mg/liter of glucose were used daily as the auxiliary substrate. Microorganisms consume auxiliary substrate as the energy source to sustain the dechlorinating capability rather than the carbon source to reproduce, thereby limiting the dechlorinating capabilities of microorganism.

The rates and extent of dechlorination of CT and TCA by the anaerobic consortia were found to be greater at the top than at the bottom of the column. Almost no chlorinated hydrocarbon was dechlorinated at the bottom in the test period. It is likely that either the bacteria were not transported to the bottom of the column or that the cells transported were inactive (Devare and Alexander, 1995). In this study, a significant amount of bacteria was observed at the bottom of the column, depicting that the cells transported were inactive. Wei (1992) demonstrated that supplementing the substrate at a downstream point 39 cm from the inlet can create a spot of desirable high microbial activity. This suggests that better substrate supplementing can enhance the remediation efficiency of groundwaters contaminated with chlorinated hydrocarbons.

Sensitivity analysis

The results of sensitivity analysis indicate that microorganisms tend to accumulate on the top of the column and the peak occurs in the first 1.5 cm of the column coupled with the rapidly mineralization of supplemental substrate. The equilibrium distribution constant of microorganisms (k_x), auxiliary substrate (C_p), decay coefficient (b) and yield coefficient of microorganisms (Y) are the crucial factors influencing the distribution of microorganisms and dechlorination of chlorinated hydrocarbons. k_x is the most important parameter in determining the distribution pattern of microorganisms. As illustrated in Fig. 6(a), different distribution patterns between the total and

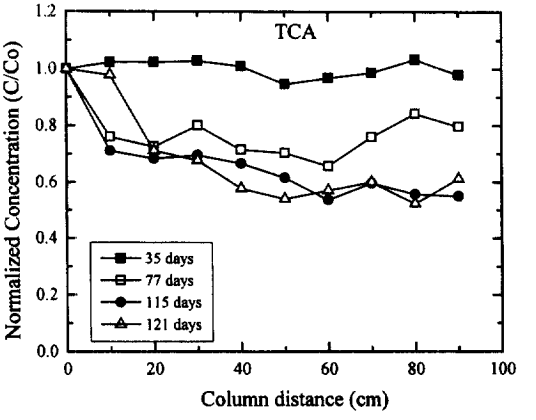

Fig. 5. Biotransformation of TCA with the amendment of 50 mg/liter glucose as supplemental substrate.

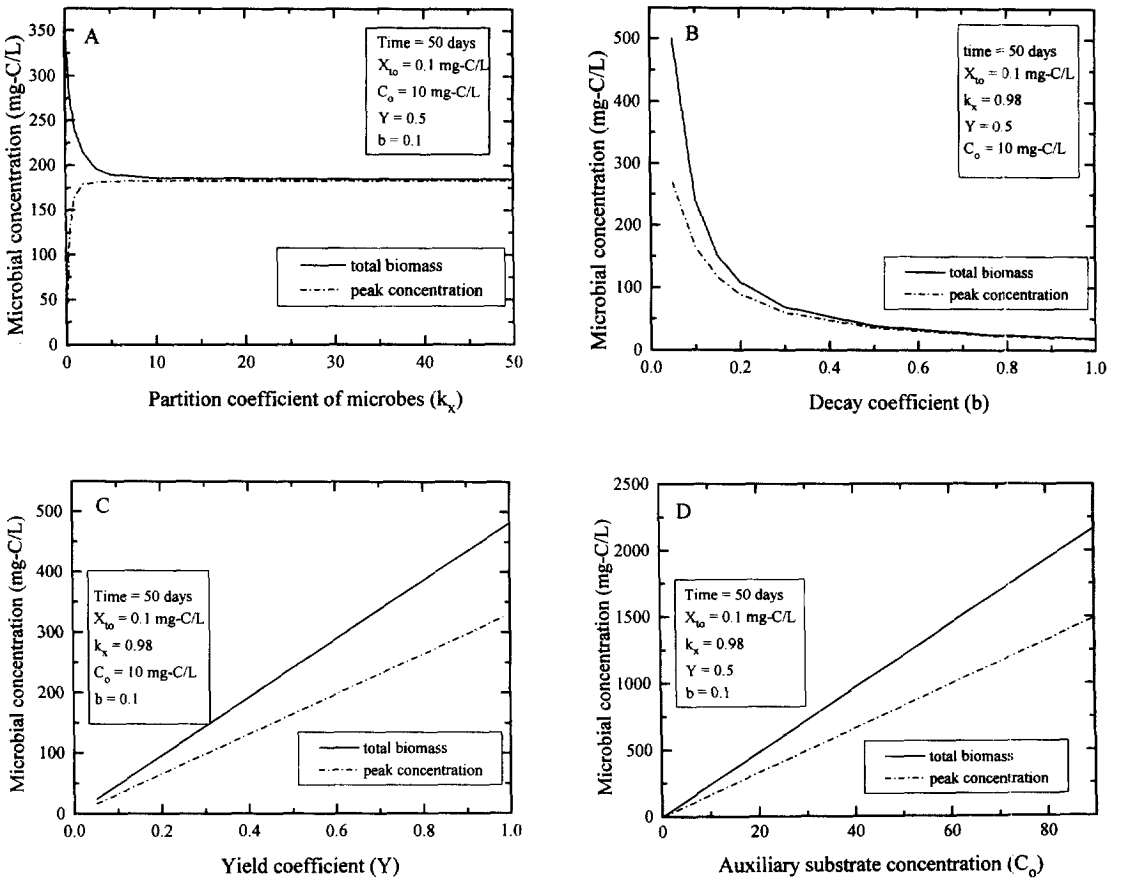

Fig. 6. Sensitivity analyses of biological parameters used in the partitioning model. The concentration profile of microorganisms are functions of biological parameters.

peak microbial concentrations were observed at k_x low value, whereas the total and peak microbial concentrations were almost the same when k_x exceeded 10. MacQuarrie *et al.* (1990) reported that the value of the microbial retardation factor could vary from 50 to 5000 without significantly affecting the xenobiotic concentration. This result indicates that free-living microorganisms are predominant at low k_x, whereas most of the bacteria can be considered as an attached biofilm at high k_x value, which is consistent with the field observations (Harvey *et al.*, 1984; Hickman and Novak, 1989).

Unlike k_x, C_p, b and Y mainly influence the total biomass retained in the column rather than the distribution pattern of microorganisms. As depicted in Fig. 6(b), the microbial concentration decreased rapidly when b increased from 0.05 to 0.2 and was almost the same when b exceeded 0.5. Also, the total and peak microbial concentrations increased linearly with an increase of C_p and Y (Fig. 6c, d). The similar distribution pattern of the total and peak microbial concentrations depicts that the total biomass was mainly from the attached biofilm. Moreover, a four-fold difference of the total biomass was observed between C_p and Y, depicting that C_p is more sensitive than Y in increasing the total biomass in the column.

Sensitivity analysis results demonstrated that the dispersion–advection parameters were only reflected in a spreading of the pollutant concentration front as it moves through the porous media. This suggests that biotransformation rates are limited by the reaction rate rather than mass transport. For large-scale subsurface contamination with low active organism concentrations and slow groundwater movement, a complex biological model may be unnecessary to describe biotransformation rates (Bouwer and McCarty, 1984). Moreover, Yates and Enfield (1989) described the transport of dissolved substances with second-order reaction and obtained a good agreement between experimental and simulated data. Therefore, a simple second-order kinetics used in the present study can predict the fate and transport of chlorinated hydrocarbon in porous media.

Model simulation

The macroscopic partitioning model was used to simulate the fate of chlorinated hydrocarbons under the anaerobic condition. Table 2 lists the values used in simulation. Values for the four unknown parameters, μ_m, K_s, Y and b were obtained by fitting the model results to the observed data. The other

Table 2. Kinetic parameters used in model simulation

Parameter	Value	Parameter	Value
θ	0.39 cm³/cm³	ρ_b	1.47 g/cm³
v	12.2 cm/day	α	73.2 cm²/cm³
C_{po}	22.0 μg-C/ml	C_{ho}	0.1 μg-CT/ml
X_{to}	0.1 μg-C/ml	L	100 cm
k_x	0.98 cm	k_2	0.008liters/mg/day
μ_m^*	1.4 day⁻¹	K_s^*	3.9 μg-C/ml
Y^*	0.12 μg-C/μg-C	b^*	0.02 day⁻¹

*Fitting value.

parameters were obtained from either experimental tests or empirical formula. The second-order rate constants of CT and TCA were obtained from a previous work (Doong and Wu, 1996). The growth and decay coefficients are assumed to be the same for attached and free-living microorganisms. Figure 7 presents the simulated and the observed biomass profile in porous media. The pattern of the microbial distribution reflects that the experimental results are quite good. These results indicate that the microorganisms accumulate at the beginning end of the column with the maximum total biomass of 101 mg-C/liter in 50 days. However, the simulated values are less than the observed results. Since there always exists some residual TOC in the incubating media which can be used as the carbon and energy sources for microbial growth, thereby increasing concentration of microorganisms in the column.

Model simulation results in Fig. 8 indicate that the predicted CT concentrations are all in the range close to the experimental data. This figure also reveals rapid depletion of chlorinated hydrocarbons near the inlet. The good agreement between the numerical and measured values demonstrates that the partitioning model is valid to predict the transport and fate of chlorinated hydrocarbons in the contaminated groundwaters.

The dechlorination pattern of chlorinated hydrocarbons correlated well with the distribution pattern of the microbial concentration, indicating that biological transformation is the major mechanism to eliminate the chlorinated hydrocarbons in the contaminated subsurface environments. Under anaerobic condition, the growth and decay coefficients are less significant than the concentration of substrate in describing the fate and transport of bacteria. A high concentration of auxiliary substrate input can increase the biomass and the desorption rate of bacteria, thereby enhancing the dechlorination efficiency of chlorinated hydrocarbons. However, a high concentration of substrate is expensive and can alter the physicochemical properties such as permeability, dispersivity and porosity (Taylor and Jaffe, 1990). In bioremediation practices, the growth of microorganisms is dynamic. Pilot and field studies are required to identify the effects of dechlorinating culture and supplemental electron donor on reductive dechlorination so that an accurate prediction can be made of the fate and transport of chlorinated hydrocarbons at contaminated sites.

CONCLUSIONS

Results in this study demonstrate that the fate and transport of chlorinated hydrocarbons in subsurfaces are significantly affected by microbial transformation. Simulated and experimental results in this investigation demonstrate that the behavior of chlorinated hydrocarbons in the porous media is consistent with the distribution pattern of microorganisms. Microorganisms tend to accumulate in the first 10 cm of the column and rapidly consume auxiliary substrate to sustain the dechlorinating capabilities, thereby facilitating the dechlorination

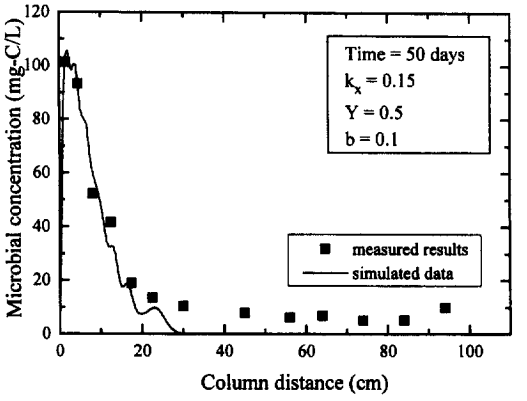

Fig. 7. Comparison of observed and simulated results in microbial density simulation at 50 days.

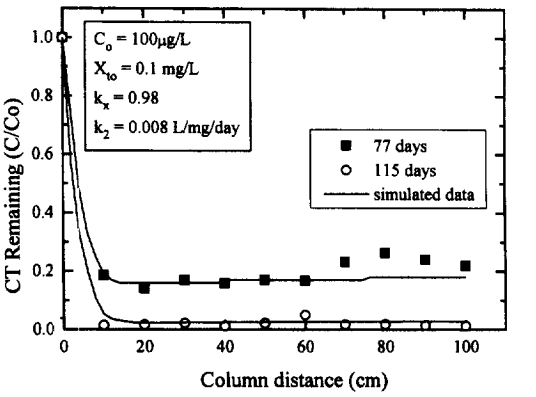

Fig. 8. Comparison of observed and simulated results in CT simulation at simulation times of 77 and 115 days.

more readily. The distribution coefficient between free-living and attached bacteria, decay and growth coefficients and auxiliary substrate concentration play prominent roles in determining the fate and transport of chlorinated hydrocarbons and microorganisms. The interaction between the auxiliary substrate and the active microorganisms has significant impact on the dechlorination of chlorinated hydrocarbons. The transport model provides the basis for describing the transport and fate of chlorinated hydrocarbons and properly selecting a remedial approach to eliminate the xenobiotics at contaminated sites.

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