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Quantitative Analysis of Transverse Bacterial Migration Induced by Chemotaxis in a Packed Column with Structured Physical Heterogeneity

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Abstract

A two-dimensional mathematical model was developed to simulate transport phenomena of chemotactic bacteria in a sand-packed column designed with structured physical heterogeneity in the presence of a localized chemical source. In contrast to mathematical models in previous research work, in which bacteria were typically treated as immobile colloids, this model incorporated a convective-like chemotaxis term to represent chemotactic migration. Consistency between experimental observation and model prediction supported the assertions that (1) dispersion-induced microbial transfer between adjacent conductive zones occurred at the interface and had little influence on bacterial transport in the bulk flow of the permeable layers and (2) the enhanced transverse bacterial migration in chemotactic experiments relative to nonchemotactic controls was mainly due to directed migration toward the chemical source zone. Based on parameter sensitivity analysis, the results showed that chemotactic parameters determined in bulk aqueous fluid were adequate to predict the microbial transport in our intermediate-scale porous media system. Additionally, the analysis of adsorption coefficient values supported the observation of a previous study that microbial deposition to the surface of porous media might be decreased under the effect of chemoattractant gradients. By quantitatively describing bacterial transport and distribution in a heterogeneous system, this mathematical model serves to advance our understanding of chemotaxis and motility effects in granular media systems and provides insights for modeling microbial transport in *in situ* microbial processes.

Keywords

porous media; chemotaxis; modeling; heterogeneity; transport; bacteria

INTRODUCTION

A substantial research effort has been devoted to describe and predict bacterial migration in natural subsurface environments. Understanding microbial transport aids in the design and implementation of *in situ* microbial applications such as bioremediation (1) and microbial enhanced oil recovery (2,3). Previous mathematical models, in which bacteria were considered as immobile colloids, have been used extensively to describe bacterial transport in both laboratory tests (4) and field-scale studies (5,6). However, in neglecting the ability of motile

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SUPPORTING INFORMATION

Detailed experimental procedures for structured column study (Figure S1) and the attractant breakthrough curve modeling work (Figure S2) are available.

bacteria to direct their own migration, these models may not completely capture the extent of migration and therefore, may incorrectly predict the distribution of microbial populations in groundwater at a particular site of interest (7).

Chemotaxis, the ability of motile bacteria to sense chemical gradients and migrate preferentially toward regions with high chemical concentrations, is believed to play an important role in enhancing biodegradation efficiency during the implementation of *in situ* bioremediation technology (8). The idea is that chemotactic microorganisms will swim toward residual pollutants or crude oil components trapped within low permeable zones, and thereby facilitate delivery of microorganisms to the source of chemical pollutants in natural environments. This hypothesis has been supported by a growing body of experimental evidence, which demonstrated that chemotaxis occurs in saturated granular media and is not dominated by convective flow at rates typical of groundwater velocities. Pedit and coworkers (9) used a capillary filled with glass beads and indicated that the accumulation of *Pseudomonas putida* G7 was higher in the capillaries initially containing naphthalene than in the control experiments without naphthalene. Wang et al.'s study (10) used a filter-chamber with a sand-packed middle compartment and found that *Pseudomonas putida* F1 migrated through the sand towards an upper compartment with a higher contaminant level and this trend was augmented by the associated microbial population growth on the pollutant. Long and Ford (11) fabricated a two-dimensional microfluidic device with a homogeneous porous matrix and reported a strong chemotactic migration of bacteria up the attractant gradient in the direction transverse to fluid flow. Consequently, given this recent experimental evidence for bacterial chemotaxis in porous media, there is a need to develop corresponding mathematical models to quantitatively determine its effect in granular media relevant to natural environments.

Numerous studies have been devoted to constructing mathematical models of this directed microbial movement at both microscopic and macroscopic scales (12,13). Keller and Segel (14) originally developed a semi-empirical continuum model of chemotaxis which successfully explained the formation of traveling bacterial bands in the capillary assays observed by Adler (15). The model, in which chemotaxis was depicted as a convective-like flow and depended on both chemical concentrations in the ambient environment and bacterial chemotaxis properties, was used widely to explain experimental results in aqueous solutions (16). Chen and coworkers (17), who studied bacterial swimming in cylindrical tubes, developed a phenomenological model to account for altered swimming trajectories in confined spaces and incorporated it into a cell balance equation to simulate chemotaxis in small diameter pores. Marx and Aitken (18) used a cell balance model with introduction of Chen et al.'s description of chemotaxis (19), satisfactorily explaining the experimental observation of *Pseudomonas putida* G7's response to naphthalene in the capillaries. By applying a similar mathematical model, Pedit and coworkers (9) reproduced the experimental data of bacterial chemotactic accumulation in capillary tubes packed with glass beads. Alternatively, Nelson and Ginn (20) used a particle-tracking method to integrate cellular dynamics simulations with colloid filtration theory to model chemotaxis in porous media, and further applied this chemotaxis model to simulate the microscopic distribution of attached bacteria on grain surfaces (21). Hilpert (22) employed a Lattice-Boltzmann (LB) numerical approach to explore chemotactic bacterial band formation in a porous medium under groundwater flow conditions. In the model, quasi-particles were used to represent individual cells moving across a grid, providing an alternative approach to correlate single cell motility to microbial population migration in a porous matrix.

Previous models for chemotaxis were validated for pore-scale systems with well-defined flows or core-scale experiments under quiescent conditions. This effort was rarely extended to simulate bench-scale or even field-scale problems, primarily because the corresponding experimental data are scarce. In this study, we developed a continuum bacterial transport model

with chemotaxis incorporated as a convective-like flow, and applied it to a laboratory-scale structured heterogeneous column with simulated groundwater flow. By fitting parameters from data in the same experimental settings reported by Wang and Ford (23), and evaluating the sensitivity of coefficient values, we tested the application of a widely-used mathematical description of chemotaxis (19) in a system that is more representative of natural groundwater systems. The simulation results also yielded details of bacterial distributions within the layers of the packed column, which were difficult to obtain experimentally. Those distributions provided further insight to the mechanisms that govern bacterial transport in complex environments.

EXPERIMENTAL SYSTEM

We used experimental data obtained by Wang and Ford (23) to evaluate our models. Detailed information regarding the materials, protocols, and experimental procedures are available in (23) and restated in Supporting Information (Part I). Briefly, a laboratory column (diameter 4.8 cm, length 15.5 cm) was packed with coarse- (710 μm diameter) and fine- grained sand (450 μm diameter) to produce a high-conductive core (1.8 cm) running parallel to the flow direction and a surrounding low-conductive annulus (Fig. 3A), a structure similar to Saiers et al. (24) and Morley et al. (25). A chemoattractant source was placed along the central axis of the column to mimic contaminants trapped in the heterogeneous subsurface. De-ionized water was pumped through the column at velocities comparable to those of groundwater. A pulse of bacteria was injected into the column and bacterial concentrations in the effluent were monitored over time. The breakthrough curves of *Escherichia coli* HCB1 in the presence of α -methylaspartate (α -mASP, 0.1 mM, initially), used as a model organism for chemotaxis studies, were compared to its no-attractant controls where sodium chloride was substituted for the chemoattractant under a flow rate of 5.1 m/d. Nitrate was used as a conservative tracer concurrently with bacterial injectates.

MATHEMATICAL MODEL

Advective-Dispersive Bacteria/Colloid Transport

The conservation equation for bacterial transport in the aqueous phase of a porous medium was modified by inserting a convection-like chemotaxis term into the colloid transport model

$$\frac{\partial b}{\partial t} + \frac{\rho_b}{\varepsilon} \frac{\partial s}{\partial t} = \vec{\nabla} \cdot (\mathbf{D}_b \vec{\nabla} b) - \vec{\nabla} \cdot [(\vec{V} + \vec{V}_c)b] \quad (1)$$

in which b (cells/mL) is the suspended bacterial concentration, s (cells/g) is the bacterial abundance associated with the solid surface, ρ_b (g/mL) is the bed density, ε (unitless) is the porosity, $\mathbf{D}_b$ (cm^2/s) is the hydrodynamic dispersion tensor, $\vec{V}$ (m/d) is the pore velocity of the fluid, and $\vec{V}_c$ (m/d) is the chemotactic velocity, quantifying the chemotaxis-induced microbial transport. The term $\partial s/\partial t$ represents bacterial retention in the porous medium, a function largely dependent on local physiochemical characteristics and bacterial abundances. Microbial growth and inactivation were assumed negligible due to the short residence time of the column experiments. The dispersion tensor $\mathbf{D}_b$ can be fully described by the longitudinal dispersion coefficient D_{bL} and the transverse dispersion coefficient D_{br} when each flow layer is treated as an isotropic homogeneous medium. Both dispersion coefficients are constituted by two components as follows

$$\begin{aligned} D_{bL} &= \alpha_L V + \frac{D_{0,eff}}{\varepsilon} \\ D_{bT} &= \alpha_T V + \frac{D_{0,eff}}{\varepsilon} \end{aligned} \quad (2)$$

where α_L (m) and α_T (m) are longitudinal and transverse dispersivities respectively, accounting for hydrodynamic characteristics of the system, and $D_{0,eff}$ (cm²/s) is the effective coefficient for diffusion of microbes, which is related to the bacterial random motility coefficient D_0 (cm²/s) in the bulk liquid phase and the tortuosity τ (unitless) by

$$\frac{D_{0,eff}}{\varepsilon} = \frac{D_0}{\tau} \quad (3)$$

The chemotactic velocity $\vec{V}_c$ (m/d) was calculated according to the expression (19,22)

$$\vec{V}_c = \frac{2v}{3} \tanh \left(\frac{\chi_{o,eff}}{2v\varepsilon} \frac{K_c}{(K_c + a)^2} \left| \vec{\nabla} \cdot a \right| \right) \frac{\vec{\nabla} \cdot a}{\left| \vec{\nabla} \cdot a \right|} \quad (4)$$

in which v (m/s) represents the swimming velocity of the motile bacteria, $\chi_{o,eff}$ (cm²/s) is the effective chemotactic sensitivity parameter in a porous medium and K_c (mM) is the chemotaxis receptor constant.

We used a first-order equilibrium and kinetic adsorption term to mathematically describe the interactions of colloids with solid surfaces (5):

$$\frac{\rho_b}{\varepsilon} \frac{\partial s}{\partial t} = k_a b - k_d s \quad (5)$$

in which k_a (s⁻¹) and k_d (g/mL · s⁻¹) are adsorption and desorption rate coefficients, respectively. Due to the successful application of a clean bed approximation for bacterial transport in homogeneous columns in Wang and Ford's study (Supporting Information) (23), Eqn 5 was reduced to

$$\frac{\rho_b}{\varepsilon} \frac{\partial s}{\partial t} = k_a b \quad (6)$$

Consequently, the conservation equation for various colloids (chemotactic bacteria, nonchemotactic bacteria, and nonmotile microspheres) in a porous medium was simplified to

$$\frac{\partial b}{\partial t} = \vec{\nabla} \cdot (\mathbf{D}_b \vec{\nabla} b) - \vec{\nabla} \cdot (\vec{V} + \vec{V}_c) b - k_a b \quad (7)$$

Similarly, the chemoattractant transport equation with terms for dispersion and advection was written as

$$\frac{\partial a}{\partial t} = \vec{\nabla} \cdot (\mathbf{D}_a \vec{\nabla} a) - \vec{\nabla} \cdot (\vec{V} a) \quad (8)$$

where a (mM) is the attractant concentration.

For the two boundaries, the first one at the interface between attractant source and porous medium r_i (cm) and the second one at the outer surface of the column R (cm), no-flux conditions were applied to the model equations according to

$$-D_{br} \frac{\partial b}{\partial r} + b V_{cr} = 0 \quad (r = r_i, R) \quad (9)$$

where V_{cr} (m/d) is the radial chemotactic velocity. Boundary conditions for the attractant concentration were given by

$$\begin{aligned} -D_{ar} \frac{\partial a}{\partial r} &= 0 & (r=R) \\ a &= a_0(t) & (r=r_i) \end{aligned} \quad (10)$$

in which D_{ar} (cm²/s) is the attractant transverse dispersion coefficient and $a_0(t)$ is the attractant source concentration which is decreasing with time due to the continuous mass exchange with the ambient environment. The change of $a_0(t)$ was simulated using a function that decreased exponentially, the equation for which was obtained by fitting it with the measured attractant breakthrough curve (detailed description in Supporting Information). The introduction of bacteria and tracers were modeled as constant flux at the column inlet over the time period of the injections.

Structured Heterogeneity

The velocity profile of groundwater bulk flow in the heterogeneous saturated column is determined by Darcy's law, which is dependent on the pressure field p (Pa) and hydraulic conductivity tensor $\mathbf{K}$ (m/s) (27)

$$\vec{V} = -\mathbf{K} \nabla p \quad (11)$$

The structured heterogeneity in the packed column was represented in the model as two domains with contrasting uniform hydraulic conductivities. The bulk fluid velocity $\mathbf{V} = (U, 0, 0)$ was different in each layer: U_1 and U_2 represented the pore velocity in the inner core and outer annulus, respectively. Since a fixed pressure head was maintained at both ends of the column and a constant flow rate was applied, the magnitude of velocities was determined by the ratio of the two layers' conductivities ($U_1/U_2 = K_1/K_2$). Other parameters that characterized the physical properties of the porous medium or were dependent on velocity were also specific to each domain. A thin interfacial layer with thickness Δr was used to reconcile the continuous change of coefficient values between the two adjacent flow zones.

Eqns. 7 and 8 were solved numerically in MATLAB (Version 7.6, MathWorks) using a fully implicit, finite difference scheme (10). Input parameters included physical properties of the column, such as the column length $L = 15.5$ cm, the radius of the agar core (source of the

attractant) $r_i = 0.3$ cm, the coarse medium core radius $R_i = 0.9$ cm, the column radius $R = 2.4$ cm, the interfacial thickness $\Delta r = 0.1$ cm, the porosity $\varepsilon = 0.43$ and the flow rate $V = 5.1$ m/d. Transport coefficient values used in the numerical solutions are presented in Table I. They were obtained by minimizing the mean squared error between experimental data and simulated output. Output from simulations to match the tracer nitrate breakthrough curves (BTCs) was used to evaluate the essential hydrodynamic parameters. The fundamental transport properties of bacteria such as dispersion and retention were quantified by fitting the model output to the bacterial data from control experiments. Then these property values were applied in the chemotactic bacterial models to elucidate the magnitude and significance of chemotaxis.

RESULTS AND DISCUSSION

Transverse Dispersion Mixing

A single pulse injection into the column yielded a breakthrough curve (BTC) with two characteristic peaks. Fig. 1 illustrates the characteristic double peak in the BTC for the conservative tracer. The first peak corresponds to mass transported through the inner fast-flow core and the second peak corresponds to mass from the outer slow-flow annulus, each of which reflects the unique hydrodynamic conditions of the corresponding layer. Bacterial BTCs demonstrated this same double-peak characteristic for *E. coli* HCB1 in Fig. 2A. Due to microbial deposition in saturated granular media, the bacterial data exhibited lower peak heights relative to the corresponding tracer. The good agreement between the mathematical model and experimental data revealed the successful application of our 2-dimensional models. The fitted parameter values for *E. coli* are listed in Table I.

Based on the size difference between microbial colloids and nitrate tracer, we expected to see differences in breakthrough times. It has been well recognized that size exclusion may cause an apparent accelerated colloid velocity (28) and thus induce an early appearance of colloids in the effluent solutions compared to conservative tracers (29). The unexpected coincidence of the peak arrival time for bacteria and tracer might be due to the short length of the tested column. However, we did observe that the longitudinal dispersion coefficients for *E. coli* were approximately two-fold larger than the corresponding tracers at low flow layer. Thus, the size exclusion effect might provoke a greater spread in the first inclining curve of microbial breakthrough, and a kinetic adsorption-desorption process, which was not taken into account in the model for the sake of simplicity, may contribute to a longer tail in the breakthrough curves of colloids (30). A combination of these factors would result in a larger magnitude of the apparent longitudinal dispersion for microorganisms and microspheres. The same trend for the bacterial strain was observed in column studies with a uniform-sized packing material (data not shown).

Dispersion-induced mass transfer also occurred to a small degree at the interface between adjacent conductive zones. The feature in the BTC's that reflects this mass transfer process is the flat portion (saddle) between the two peaks observed for the tracer (Fig. 1) and control bacteria (Fig. 2A). The juxtaposition of two layers with different particle sizes creates heterogeneity that facilitates mass exchange at the interface (31). In previous studies, BTCs through multiple permeable zones with different hydraulic conductivities were calculated by linear addition of contributions from each zone, particularly in field tests with ill-defined aquifer characteristics such as Harvey and Garabedian's study (5). However, by neglecting the exchange between layers, mass transfer information in the transverse direction was lost. For example, simply adding independent transport equations from two permeable zones did not capture the saddle feature in the breakthrough curves observed in the experiments (23).

The similar scale of fitted transverse dispersion coefficients between tracer and colloids listed in Table I suggested a similar magnitude of transverse mixing for each of them. This result

supported Morley et al.'s (25) conclusion that a conservative tracer was adequate to represent transverse dispersion for bacteria. Note however, that it is possible that the contribution to transverse dispersion was so small relative to other mass transfer processes that the large physical size difference between tracer and microbes could be totally neglected. The small magnitude of the transverse dispersion coefficient in this study supported the conclusion that only an amount of mass was exchanged between the two adjacent flow layers by a dispersive mechanism. The majority of the mass was transported longitudinally by convective flow and remained within a single layer.

Transverse directed migration

The notable difference in bacterial BTCs between the chemotactic experiment (Fig. 2B) and the control one (Fig. 2A) pointed to another transport mechanism to drive microbes into the inner flow layer besides transverse dispersion, which we attributed to chemotaxis. The presence of an attractant source along the column centerline gave rise to a radial chemical gradient, which formed due to diffusion. In response to a higher chemoattractant concentration towards the center, microorganisms, which originally entered the low permeability zone, swam across the interface to the high velocity inner region, which led to a change in bacterial recoveries exiting from those two flow layers. The recovery difference in each peak of the bacterial breakthrough curves between chemotactic bacteria and controls was captured successfully by our model upon inclusion of the chemotaxis term.

The model further elucidated the spatial distribution of bacteria in the experimental system. Due to the difficulty in obtaining the corresponding experimental data, our two-dimensional mathematical model was extremely valuable in helping understand how the bacterial distributions within the column were related to the measured effluent concentrations. As indicated in Fig. 3B, the simulated *E. coli* two-dimensional distributions in granular media for both control and chemotaxis experiments revealed that the system heterogeneity and chemotaxis effects worked together to induce the observed bacterial migration. The left boundary of the two-dimensional image represents the interface between attractant source and granular media in the column. The left side of the image is the coarse sand layer, where the bacterial population transports faster from the inlet of the column (bottom of image) to the outlet (top) to yield the first peak in the BTC. The right side of the image is the fine sand layer. The mass transported through this layer corresponds to the second peak in the BTC. Although the breakthrough peaks moved through the column at the same velocity, the radial distributions of chemotactic bacteria and the no-attractant controls were different. Chemotactic microorganisms concentrated in regions closest to the chemoattractant source: near the left boundary of the image and near the interface between the two sand layers. This chemotactic response led to a nonuniform distribution of the microbial population in the two flow layers as more bacteria were directed to the inner faster regions near the attractant source. The nonuniform bacterial distribution was observed throughout the duration of the experiment in both layers as illustrated in the four sequential 2-dimensional images in Figure 3B. This focusing of bacterial populations near the contaminant source implies the possibility of even faster degradation rates in bioremediation applications which cannot be estimated by simply considering the general bacterial recovery changes in different flow layers from the BTCs. Differences between chemotactic and control distribution in the first several minutes also suggested a short time scale for microorganisms to exhibit chemotaxis. Previous chemotaxis assays in aqueous solutions typically demonstrated the bacterial responses in <10 minutes, such as capillary assays (15), stopped-flow diffusion chamber assays (16), and agarose plug assays (32). Wang and Ford's study (10) in porous media revealed that chemotaxis had a smaller time scale compared to growth when the chemoattractant also served as a growth substrate.

Sensitivity analysis to reveal other chemotactic influences

A sensitivity analysis was applied to the fitted parameters in simulation results of *E. coli* to determine the importance of chemotaxis term in the model and elucidate the impact of chemotaxis on other microbial processes such as adsorption. Inspection of Eqn. 4 revealed that the key parameters which determine the magnitude of chemotactic response in porous media are the effective chemotaxis sensitivity coefficient $\chi_{o,eff}$ and the chemotaxis receptor constant K_c . The chemotaxis receptor constant characterizes the chemosensory mechanism that relates information about the external chemical stimulus to the motors that control the rotation of flagella. As a representative property of a microbial strain and chemoattractant system, the value of K_c is usually assumed to be independent of the external physical environment. In contrast, the effective chemotactic sensitivity coefficient $\chi_{o,eff}$, a parameter to quantify the strength of chemotactic response based on directed microbial movement, lumps together effects from both bacterial swimming properties and the impact of the surrounding matrix. Therefore, we used literature values of K_c but fit values of $\chi_{o,eff}$ in our model to experimental data.

While substantial effort has been devoted to the accurate measurement of chemotaxis sensitivity in aqueous solutions, the few reported values in porous media span a wide range. The chemotactic sensitivity of *E. coli* to α -methylaspartate was reported as $2.4 \times 10^{-4} \text{ cm/s}^2$ (33) and $4.1 \times 10^{-4} \text{ cm/s}^2$ (34) in bulk aqueous solutions while the coefficient for its response to L-aspartate was reported as $5.7 \times 10^{-4} \text{ cm/s}^2$ in a glass capillary array with 50 μm diameter pores and $13 \times 10^{-4} \text{ cm/s}^2$ in an array with 10 μm diameter pores (35). While Pedit *et al.* reported a decreased chemotactic response in a bead-packed capillary (9), Long and Ford (11) noted a highly enhanced chemotactic response in their 2-D etched porous matrix, in which the chemotactic sensitivity was estimated to be two orders of magnitude higher than the previously reported one in aqueous solutions. In our study, the fitted $\chi_{o,eff}$ value for *E. coli* to α -methylaspartate was $8.0 \times 10^{-4} \text{ cm/s}^2$ as listed in Table I. The similar range of values predicted by our model in porous media and those reported in the literature for aqueous solutions suggested that the presence of the porous media did not have a significant effect on the magnitude of chemotactic sensitivity coefficient in this particular experimental configuration. Results from the sensitivity analysis of $\chi_{o,eff}$ for *E. coli* are shown in Fig. 4a. Reducing the value by cutting it in half resulted in a $\sim 15\%$ increase of the second peak height and no apparent change in the first peak of the *E. coli* BTC. Increasing the value reversed this trend. The unbalanced change in mass of the two peaks was due to the large microbial irreversible attachment in the inner coarse layer. Mass recovery was checked for all conditions when no attachment term was applied, with the result that the mass was conserved. The small differences observed among fitted curves within the range of parameter values implied that values of $\chi_{o,eff}$ determined in bulk aqueous fluid could be used to estimate the microbial transport in our intermediate-scale porous media system. The sensitivity analysis results for another important parameter, the irreversible adsorption coefficient k_a , are shown in Fig. 4b. As listed in Table I, the value of k_a in the inner coarse layer fitted for chemotactic *E. coli* was just 40% of the one for nonchemotactic controls. This difference was significant in determining the first peak height in bacterial BTCs. This mathematical analysis supported the assertion that chemotaxis might decrease microbial adsorption to media surfaces. It was not surprising when taking into account the attractant effects on single microorganism swimming behaviors, which induced longer swimming length and less frequent reorientation (36). The changes in swimming pathways influence the interaction between bacteria and the porous matrix. McClaine and Ford (37) observed that the smooth-swimming *E. coli* mutant attached less to a glass surface than the wide-type with intermittent tumbles. Velasco-Casal *et al.* (38) noted the reduced deposition of strain *P. putida* G7 in a packed column in the presence of chemoattractant naphthalene. Therefore, the microbial population that was close to the attractant source might undergo a

significant chemical gradient's impact, which may induce an observable mass increase in the first peak of microbial BTC.

Implications for Microbial Transport Models

The good agreement between the two-dimensional mathematical model and the experimental data illustrated a successful application of the model with the chemotaxis expression proposed by Chen et al. (19). Under conditions relevant to most natural porous media systems, chemotaxis may contribute in a significant way to dispersion, especially in the directions transverse to groundwater flow. This directed microbial migration controls the spatial distribution of microorganisms in both aqueous and soil phases, which directly correlates to the efficiency of microbial processes. Therefore, it may be important to include the description of chemotaxis in macroscopic microbial transport models in order to accurately capture the microorganism transport and adsorbed bacteria distributions in microbial processes applied in natural and engineered systems.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.

BTC of the nitrate tracer at the flow velocity of 5.1 m/d. Nitrate concentrations are normalized to its initial concentration in the injectate. The sparse dots represent experimental data from five independent trials and the bold line is the fitted simulated result from the mathematical model using the parameters listed in Table I.

Figure 2.

E. coli HCB1 BTCs for (A) nonchemotactic controls and (B) chemotaxis experiments at 5.1 m/d with symbols as follows: • experimental data for nonchemotactic controls, --- simulated result for nonchemotactic controls, + experimental data for chemotactic bacteria, and - simulated result for chemotactic bacteria.

Figure 3.

E. coli HCB1 transport at 5.1 m/d. (A) axial cross-section of the two conductive zones in the structured column with the simulated region for bacterial concentration distribution indicated. (B) Two-dimensional distributions of aqueous bacterial concentrations in two permeable layers at dimensionless times equals to 0.1, 0.25, 0.5, 1 pore volume (PV). Note that the scale bar for intensity has different maximum values for each of the experimental times. Figure (A) is adapted from Wang and Ford (23)

Figure 4. Sensitivity analysis of the *E. coli* transport parameters using coefficient values in Table 1 for the other parameters. The sparse points (+) are the experimental data of chemotactic bacteria. (A) Sensitivity analysis of $\chi_{o,eff}$, the effective chemotactic sensitivity coefficient. (B) Sensitivity analysis of k_{a1} , the deposition coefficient in the coarse sand layer.

Table IFitted Transport Parameters for Tracer Nitrate and *E. coli* HCB1 at 5.1 m/d

Parameters	Tracer	<i>E. coli</i>
K_1/K_2	4.3	4.0
$D_{z1}(\text{cm}^2/\text{s})$	1.1×10^{-2}	1.1×10^{-2}
$D_{z2}(\text{cm}^2/\text{s})$	2.5×10^{-4}	4.3×10^{-4}
$D_{r1}(\text{cm}^2/\text{s})$	3.6×10^{-5}	3.4×10^{-5}
$D_{r2}(\text{cm}^2/\text{s})$	9.2×10^{-6}	9.5×10^{-6}
$K_{a1}(\text{h}^{-1})$		$2.12^1, 0.85^2$
$K_{a2}(\text{h}^{-1})$		0.23
$x_{0,eff}(\text{cm}^2/\text{s})$		8.0×10^{-4}
$K_c(\text{mM})$		0.125^3

Note: For all parameters, subscript 1 refers to the inner coarse layer and subscript 2 refers to the outer fine annulus.

¹ applied in the model of no-attractant control simulation

² applied in the model of chemotactic bacterial simulation

³ Mesibov *et al.* (39)