Random Walk Calculations for Bacterial Migration in Porous Media

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ABSTRACT Bacterial migration is important in understanding many practical problems ranging from disease pathogenesis to the bioremediation of hazardous waste in the environment. Our laboratory has been successful in quantifying bacterial migration in fluid media through experiment and the use of population balance equations and cellular level simulations that incorporate parameters based on a fundamental description of the microscopic motion of bacteria. The present work is part of an effort to extend these results to bacterial migration in porous media. Random walk algorithms have been used successfully to date in nonbiological contexts to obtain the diffusion coefficient for disordered continuum problems. This approach has been used here to describe bacterial motility. We have generated model porous media using molecular dynamics simulations applied to a fluid with equal sized spheres. The porosity is varied by allowing different degrees of sphere overlap. A random walk algorithm is applied to simulate bacterial migration, and the Einstein relation is used to calculate the effective bacterial diffusion coefficient. The tortuosity as a function of particle size is calculated and compared with available experimental results of migration of *Pseudomonas putida* in sand columns. Tortuosity increases with decreasing obstacle diameter, which is in agreement with the experimental results.

INTRODUCTION

Modern production of synthetic organic compounds has resulted in their accumulation throughout the environment (Bouwer, 1992). Much of this organic waste originates from solvents, plastics, dyes, feed stocks, fertilizers, and fuels and their additives. It is costing the United States billions of dollars to remediate existing ground water and soil sites that are polluted (Rittmann et al., 1993). In situ bioremediation, a method of restoring contaminated soils using bacteria to degrade pollutants, is of interest because it may prove more cost-effective than traditional technologies such as incineration and pump and treat methods.

The aim of our research is to develop a theoretical model for bacterial migration within contaminated aquifers incorporating the properties of the bacteria, the soil matrix, and the contaminant. This would aid in developing a quantitative understanding of the processes involved and provide a method to assist engineers in designing effective remediation strategies.

The soil bacteria *Pseudomonas putida* propel themselves through their surrounding media by rotating flagella that form a tuft at one end of their body (Harwood et al., 1989). A single cell traces a path that consists of a series of runs interrupted by changes in direction. As with *Escherichia coli*, the changes in direction are initiated by a reversal in the rotational direction of the flagellar motors of the bacteria. However, unlike *E. coli*, *P. putida* do not exhibit tumbling behavior between changes of direction (Harwood et al., 1989). In the absence of a chemical gradient, this swimming pattern resembles a three-dimensional random walk similar to Brownian motion in molecular diffusion, except that changes in direction are due to the reversal of flagellar rotation and not molecular collisions. This behavior is referred to as random motility.

One question that arises, the subject of this paper, is: To what extent does the morphology of the soil matrix affect the random motility of the bacteria? Measurements of bacterial penetration in sand columns with uniform particle size performed in our laboratory have shown that the effective random motility decreases with decreasing particle diameter (Barton, 1994). This dependence is quite dramatic, with a twofold change in particle size resulting in as much as a fourfold change in random motility. These experiments are performed with particles having a narrow distribution in diameter (i.e., approximately monodisperse). For random packings of monodisperse spheres, the porosity has been shown to be effectively independent of sphere size (Huizenga and Smith, 1986). Thus, the experimental studies suggest that obstacle diameter has an effect on the cell motility independent of the porosity of the system (Barton, 1994).

Sahimi and Jue (1989) simulated macromolecular diffusion in a disordered porous medium, which corresponds to the Brownian motion of macromolecules found in a real system. They found a sharp dependence of the effective diffusion coefficient on the mean pore diameter of the medium. Thus, it is possible that the average effective random motility of the bacteria is a function of the pore morphology.

Frymier et al. (1993) used a random walk algorithm to simulate random motility in bulk systems using a series of straight line segments (runs) interrupted by tumbles with

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changes in direction. A modification of this method is used here to study motility within a porous matrix. Note that bacterial migration in a porous medium differs in several ways from the system modeled by Sahimi and Jue (1989). They consider bulk diffusion where the molecular mean free path is small compared with the mean pore diameter. At the other extreme, Knudsen diffusion, as found in gaseous diffusion through narrow pores, occurs when the natural molecular mean free path is much greater than the mean pore diameter. For bacterial migration in a typical porous media used to model sandy aquifers, the process lies in the transition between these two extremes because the bacterial mean free path is of the same order as the magnitude of the mean pore diameter. The mean free path is approximately 0.01 cm for *P. putida* (Harwood et al., 1989), whereas the mean pore diameter in the sand column experiments ranges from 0.004–0.03 cm. This is based on the relationship $\sigma_p/\sigma = 0.39$, where σ is the obstacle diameter and σ_p is the mean pore diameter, presented by Huizenga and Smith (1986) with mean obstacle diameters σ = 0.01–0.08 cm (Barton, 1994). Because there is a distribution of path lengths about the mean pore diameter, we expect a combination of bulk diffusion and Knudsen diffusion.

There are two further differences between Brownian motion of molecules and bacterial motility. First, bacteria such as *E. coli* have a small bias to persist in their direction of motion after tumbling, resulting in a nonuniform random turn angle distribution, whereas in the Brownian motion of molecules the direction after collisions has a uniform random turn angle distribution. Second, the change in direction made by the cell takes a finite time, whereas in Brownian motion a change in direction is considered to be instantaneous. Thus, one cannot simply infer results from the previous work of Sahimi and Jue (1989) for molecules to the behavior of bacteria.

The aim of this work is to use a random walk algorithm specifically designed to model bacterial migration in a constructed porous matrix to investigate the effect of the obstacle diameter on the effective random motility coefficient of bacteria and to compare the results with experimental measurements.

MATERIALS AND METHODS

Generation of a model porous medium

A model porous medium is generated in three dimensions using a simulation "box" filled with "spheres" of equal size that act as obstacles. A random configuration of the spheres is created using a molecular dynamics simulation of hard spheres, each with unit diameter (Allen and Tildesley, 1987). The free volume (or porosity, ϕ) of the medium is adjusted by increasing all sphere diameters by a fixed amount, and the porosity is calculated using a Monte Carlo algorithm. Overlap of the spheres is allowed, and the final configuration resembles the penetrable-concentric-shell (or "cherry pit") model introduced by Torquato (1991). However, the amount of overlap is minimal for the fixed porosity of 0.37 at which all of the simulations are run. Each of 2048 spheres is given an equal diameter in the micrometer range. By varying only the size of the system, the porosity can be kept constant for a range of obstacle diameters.

Simulation methodology

Initially, 1000 cells are placed on a set of points uniformly distributed throughout the pore space. Each cell is given a random direction vector. In this way, each cell traverses a unique path. In similar simulations of gas diffusion in porous media, it has been shown that this method yields accurate diffusivity measures if the average tracer displacement covers a minimum distance of 10 diameters (Reyes and Iglesia, 1991). For this study, a distance equal to five obstacle diameters was found to be sufficient. However, many of the simulations were run for distances exceeding 10 diameters.

The logic diagram in Fig. 1 summarizes the simulation methodology, which is a modification of the cellular dynamics algorithm developed by Frymier et al. (1993) for bulk systems combined with elements of the algorithm of Kim and Torquato (1992) developed for gaseous diffusion in porous media. After initialization, motility of a bacterial population is simulated by performing a number of calculations on each bacterium separately. First, it is determined whether the cell changes direction. This depends on a probability β_0, which is specific to the species of bacteria under consideration. Second, if a new direction is required, then it is chosen using the method of Frymier et al. (1993); otherwise, the original direction is maintained. Third, the new position is calculated from the direction vector, the swimming speed, and the time step. Fourth, this new position is checked to see whether it falls in the void fraction of the porous medium. If it does, then the change in position is made; if not, the original position is maintained. In either case, the time is incremented by the time step and the steps are repeated.

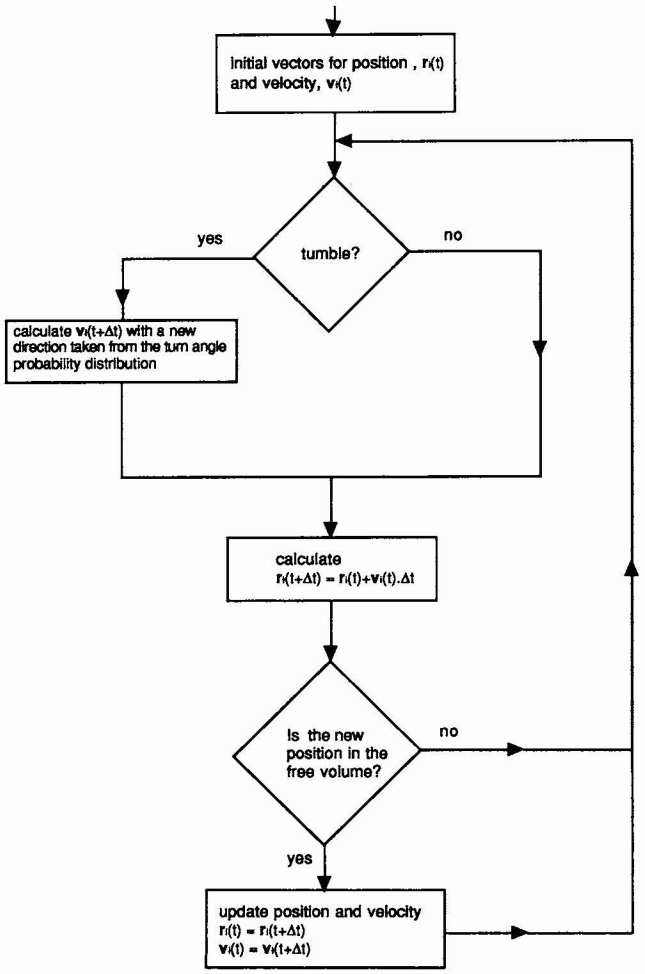

FIGURE 1 Logic diagram for the simulations.

This method gives an accurate estimate of effective diffusion in porous media as long as the simulation step is no more than 0.01 of an obstacle diameter (Schwartz and Banavar, 1989). For the present study, the time is incremented by $\Delta t = 0.01$ s (or a step length of 0.44 μm at the swimming speed of 44 μm/s), which is equal to 0.005 of the mean free run time of the simulated bacteria in the bulk (2 s, corresponding to a mean free path in the bulk of 88 μm). Because the diameters of the obstacles considered are 50 μm and higher, the time step used ensures that each simulation step is less that 0.01 of each obstacle diameter, thus meeting the criterion of Schwartz and Banavar.

Thus, if permitted in the void space, the position $\mathbf{r}_i$ of bacterium i at time $t + \Delta t$ is given by

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \nu \mathbf{s}_i \Delta t, \tag{1}$$

where ν is the three-dimensional swimming speed and $\mathbf{s}_i$ is the unit direction vector that evolves in time according to

$$\mathbf{s}_i(t + \Delta t) = \lambda_i \mathbf{s}_i(t) + (1 - \lambda_i)\mathbf{s}_{i,\text{new}}(t), \tag{2}$$

where

$$\lambda_i = \Theta[\rho_i(t + \Delta t) - \beta_0 \Delta t]. \tag{3}$$

Here ρ_i is a random number from the interval [0,1], and the new direction, $\mathbf{s}_{i,\text{new}}(t)$, is found by randomly choosing θ_i, the angle between $\mathbf{s}_i(t)$ and $\mathbf{s}_{i,\text{new}}(t)$, from a distribution of turn angles measured by us and shown in Fig. 2 and by choosing the azimuthal angle from a uniform distribution. Details on the method for choosing θ_i can be found in Frymier et al. (1993). θ is the Heaviside function, defined as

$$\Theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0. \end{cases} \tag{4}$$

Thus,

$$\begin{aligned} \lambda_i &= 1 \quad \text{if} \quad \rho_i \geq \beta_0 \Delta t \\ \lambda_i &= 0 \quad \text{if} \quad \rho_i < \beta_0 \Delta t, \end{aligned} \tag{5}$$

so that each bacterium has a probability $\beta_0 \Delta t$ of changing its direction and a probability of $(1 - \beta_0 \Delta t)$ of continuing its run.

The distribution of turn angles for *P. putida* given in Fig. 2 was measured using the tracking microscope developed by Berg and Brown (1972). Although the algorithm used to analyze the tracking data was designed for *E. coli* and not for *P. putida* specifically, the turn angle distribution of *P. putida* appears to be qualitatively different from that measured by Berg and Brown (1972) for *E. coli*. The distribution is bimodal with a higher peak near the lower angles. This indicates that each bacterium, when choosing a new direction, is most likely to choose a direction not very different from or approximately opposite to the previous direction. This behavior matches the qualitative behavior observed by one of the authors using standard microscopy.

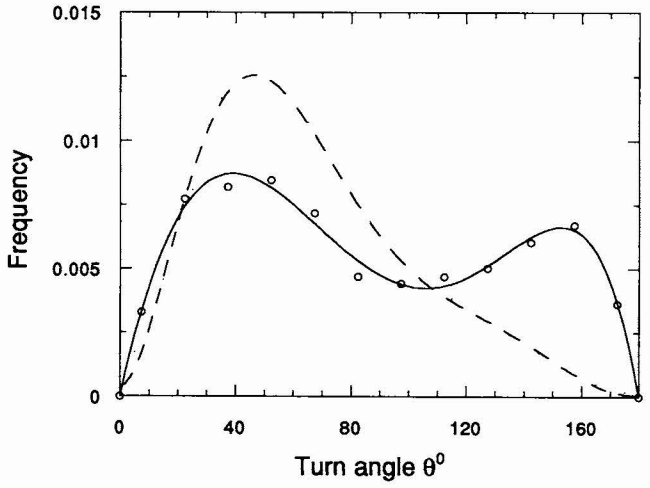

FIGURE 2 Frequency of turn angles for *P. putida* (○). The curve for *E. coli* is included for comparison (– – –) (Berg and Brown, 1972).

The random walk simulation is performed in the free volume of the model porous medium. Each bacterium is represented as a sphere with a diameter δ equal to an approximate average axial length for that species. This is included in the simulation by replacing the obstacle diameter σ with the sum of the cell diameter and the obstacle diameter ($\sigma = \sigma + \delta$) and considering the cell diameter as a point particle. Kim and Torquato (1992) have shown that solutions using these two methods of accounting for overlaps of finite sized diffusing particles with the matrix are equivalent.

Periodic boundary conditions are implemented for both the porous matrix and the bacterial motion such that when a cell moves out of the simulation box it is repositioned just inside the opposite side. In this way, cell number density is conserved within the box.

The cell swimming speed ($\nu = 44$ μm/s) and the direction change probability ($\beta_0 = 0.5$/s) are average values for *P. putida* reported by Harwood et al. (1989). Variations in swimming speed are unimportant for this study because this variable scales out of the equation of interest (see below). Variations in β_0 are considered and represent the largest variation reported by Harwood et al. (1989). A value of $\beta_0 = 0.1$ represents the value measured for cells responding to a temporal gradient after the addition of a chemoattractant. The duration of a change in direction ($t_0 = 0.025$ s) is an average value of those reported by Harwood et al. (1989). Parameter values for the simulations are summarized in Table 1.

RESULTS

Random motility calculations and simulation accuracy

The random motility coefficient μ is calculated from the mean-square displacement $\Omega(t)$ of the cells after time t defined by

$$\Omega(t) = \frac{1}{N} \sum_{i=1}^{N} [\mathbf{r}_i(t) - \mathbf{r}_i(0)]^2 \tag{6}$$

and using the Einstein relation,

$$\Omega \rightarrow 6\mu t \qquad \text{as} \quad t \rightarrow \infty \tag{7}$$

In essence, the Einstein equation measures the average radial distance moved by a bacterium in time t, so that higher values of μ imply shorter times required on average to reach a given radial distance from the starting point. Equation 7 has been shown to be satisfied for $t > 2$ s when simulating the random motility of *E. coli* in bulk solution (Frymier et al., 1993) and for values of the parameters in Table 1. Furthermore, the mean-square displacement in the porous medium is also linear as shown in Fig. 3. When Eq. 7 is used for bacterial migration in bulk solution, we will denote the corresponding μ as the bulk phase random motility, μ_0. When Eq. 7 is used for bacterial migration in a porous medium, we will denote the corresponding μ as the effective random motility, μ_{eff}.

TABLE 1 A summary of parameter values used in the simulations

δ (μm)	ν (μm/s)	t_0 (s)	β_0 (s^{-1})
2	44	0.025	0.1, 0.5, 0.98

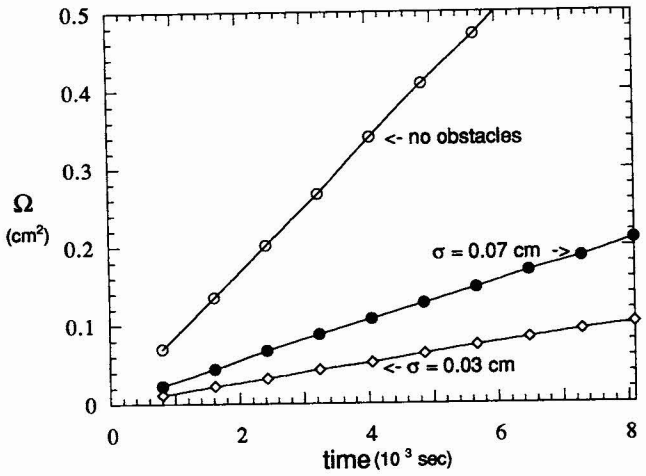

FIGURE 3 Mean-square distance of bacterial simulation traces against time in the presence and absence of a porous matrix. Two obstacle sizes are presented as indicated on the graph. Simulations were run using parameters from Table 1 and $\beta_0 = 0.5$.

The accuracy of the computer algorithm was checked using a rigorous three-point upper bound originally derived by Beran (1965) and later developed to cover a range of sphere conformations by Kim and Torquato (1992). Here the effective diffusion coefficient D_{eff} for the diffusion problem is bounded above by

$$\frac{D_{\text{eff}}}{D} \leq \phi - \frac{\phi\Phi}{(3 - \Phi - 2\zeta)}, \tag{8}$$

where ϕ and $\Phi = 1 - \phi$ are the available and unavailable volume fractions, respectively, and ζ is a three-dimensional microstructural parameter that has been investigated by Miller and Torquato (1990) and found to be well approximated by the quadratic formula

$$\zeta = 0.21068\Phi - 0.04693\Phi^2. \tag{9}$$

Kim and Torquato (1992) note that the corresponding lower bound vanishes for diffusion in a porous medium.

To compare the present algorithm with this upper bound, we used a uniform random turn angle distribution, corresponding to the case for which the bound was derived. The parameter values summarized in Table 1 were used. For a porosity such that $\phi = 0.37$ and $\Phi = 0.63$, the microstructural parameter $\zeta = 0.1141$ and $D_{\text{eff}}/D \leq 0.2730$. A comparison of our simulations for diffusion in a porous media averaged over 1000 tracers gives a value for $D_{\text{eff}}/D = 0.2671$, which falls below this upper bound.

Simulation results compared with experiment

The simulations were designed to mimic the experimental setup used by Barton (1994). In these experiments, commercially obtained silica sand is sieved into a narrow distribution of particle sizes and placed in a column with dimensions 2.5 cm in diameter and 6 cm in height. Aqueous buffer is infused throughout the column of sand, with *P. putida* included only in the bottom half of the column. Diffusion of bacteria into the upper half of the column is measured after 24 h by removing sections of the sand and performing plate counts to determine the bacterial population density profile within the sand column. To focus purely on bacterial migration, the experimental setup was designed to prevent growth (the media in which the bacteria swam contained no carbon source), eliminate flow and reduce adhesion to the porous matrix (by washing and cleaning of the sand). Accordingly, all three of these factors are ignored in the simulation.

In these experiments, the usual "tortuosity" τ lumps together the effects of diffusion in the transition regime (see discussion below) with the increase in the number of smooth swimming segments. The increase in the number of smooth swimming segments results from the obstruction by solid particles (i.e., the tortuosity of the bacterial paths imposed by the matrix). Tortuosity is thus defined as the ratio of random motility μ_0 in the bulk to the effective value in the sand column μ_{eff} accounting for excluded volume with the porosity ϕ and is written as

$$\tau = \phi \frac{\mu_0}{\mu_{\text{eff}}}. \tag{10}$$

Fig. 4 is a comparison of the simulation results, using the parameters in Table 1, with the experimental results for *P. putida* in the sand column. There is qualitative agreement between these experimental and simulated data. For both there is an overall increase in τ with decreasing obstacle size (Fig. 4). The quantitative differences may be attributed to a decay in random motility observed experimentally over 24 h, but not accounted for in the simulation.

It is of interest to see what effect variation in the probability of making a change in direction, β_0, will have on the parameter τ. Simulation results for three values of β_0 are given in Fig. 5 that represent the range of values reported by

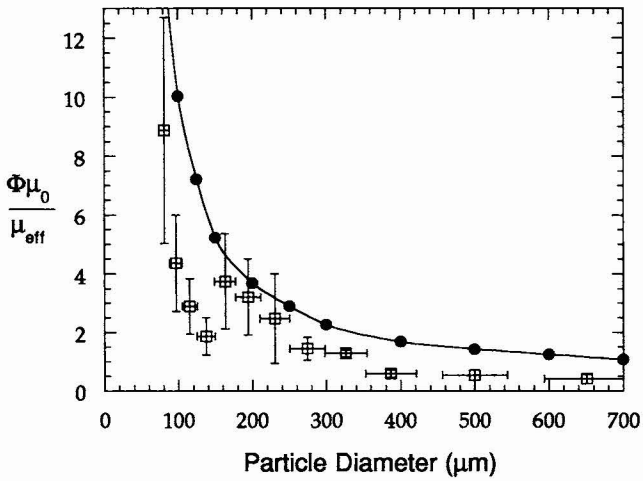

FIGURE 4 Comparison of the simulation (*circles*) and experimental data (*squares*) from Barton (1994) for tortuosity dependent on obstacle diameter. Simulations were run using parameters from Table 1 and $\beta_0 = 0.5$. Experimental error bars were calculated using SE.

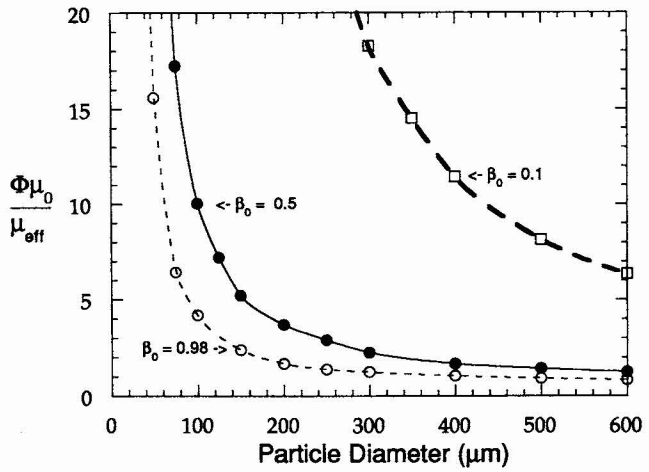

FIGURE 5 Simulation results, using parameters from Table 1, for different values of the tumbling probability β_0.

Harwood et al. (1989) in the presence and absence of chemical gradients. The average duration of a cell path length is inversely proportional to β_0. Thus, a reduction in β_0 is equivalent to an increase in the path length. With an increase in path length, one would expect the curves to be shifted to the right as seen in Fig. 5.

Harwood et al. (1989) reported probabilities for a change in direction as low as $\beta_0 = 0.1$, which corresponded to a situation for *P. putida* in a bulk aqueous phase with chemoattractant added. For the simulations in a porous matrix, this increase in β_0 significantly increases the tortuosity associated with a given particle diameter. This might explain why Barton and Ford (Barton, 1994) did not observe enhanced penetration through porous media in experiments measuring migration under the influence of a chemotactic gradient. An increase in path length, due to chemotaxis, increases the tortuosity, which counteracts the directed motion. This suggests that within the confines of the experimental situation studied by Barton (1994), chemotaxis does not enhance bacterial penetration. However, in natural situations it is likely that local chemotactic gradients within the pores, as could be expected in the vicinity of an inclusion of an insoluble or sparingly soluble contaminant material absorbed to a soil matrix, influence the migration significantly on a local level. Additionally, consumption of contaminants by bacteria creates additional attractant gradients that are explicitly excluded in the current experimental setup. Experimental and theoretical studies to probe these questions are currently underway in our laboratory.

Tortuosity

We are interested in measuring the effect of pore morphology on the bacterial migration. Transport in a porous medium is hindered primarily by the volume fraction of obstructions. However, different media can inhibit transport to varying degrees if there are differences in path space available to the tracer. The complexity of individual paths available to the cells can vary depending on the morphology of the medium. This effect of morphology on diffusion is commonly referred to as tortuosity. In practice, however, this term often includes a number of effects including path tortuosity, hydrodynamic effects, chemical interactions, and surface interactions. Thus, this paper is concerned with characterizing geometric aspects associated with the diameter of the pore relative to the bacterial path length and the tortuous nature of the pore path within the porous matrix.

Before separating out the effects of morphology on the tortuosity, one must consider the mechanism of cell diffusion within the pore space of the medium. For molecular diffusion, there are two dominant mechanisms, one depending primarily on molecular collisions and another depending primarily on molecule-surface collisions (Reyes and Iglesia, 1991). These mechanisms are referred to as bulk and Knudsen diffusion, respectively. The situation of interest here is when a combination of the two mechanisms operate, which is referred to as the transition regime.

By analogy to a common expression for molecular diffusion in a porous medium, an alternate definition of the effective tortuosity corrected for behavior in the transition region is given by

$$\tau_{corr} = \phi \frac{\mu_{trans}}{\mu_{eff}}, \tag{11}$$

where μ_{trans} is the random motility in the transition regime between Knudsen diffusion and bulk aqueous diffusion. Lovely and Dahlquist (1975) derive a relation for random motility in bulk aqueous solution given by

$$\mu_0 = \frac{\nu^2}{3\beta_0(1 - \Psi)}, \tag{12}$$

which depends on the cell swimming speed, ν, and ψ, the average value of cos φ, φ being the angle between the direction vectors before and after a change in direction. However, for *P. putida*, φ has an average value of approximately 90° (Fig. 2). With $\psi = 0$, Eq. 12 reduces to the commonly used equation for bulk diffusion, $D_b = \lambda\nu/3$ with $\lambda = \nu/\beta_0$. A corresponding equation for Knudsen diffusion (D_k) given by Reyes and Iglesia (1991) is $D_k = \sigma_p\nu/3$, so for the bacteria we have

$$\mu_k = \frac{\sigma_p \nu}{3}, \tag{13}$$

where σ_p is the mean pore diameter between obstacles. A rigorous equation for the transition between the bulk regime, and the diffusion regime for long cylindrical pores is given by the Bosanquet equation (Reyes and Iglesia, 1991):

$$D_{trans} = \frac{1}{[D_b^{-1} + D_k^{-1}]}, \tag{14}$$

where D_b is the bulk diffusion. This equation is a good predictor of gaseous diffusion in the transition regime for

a model porous medium constructed from randomly overlapping capillaries (Tomadakis and Sotirchos, 1993).

By analogy to the Bosanquet equation, we define random motility in the transition regime μ_{trans} by the following

$$\mu_{trans} = \frac{1}{[\mu_0^{-1} + \mu_k^{-1}]} = \frac{\sigma_p \nu^2}{3(\beta_0 \sigma_p + \nu)}, \quad (15)$$

where σ_p is the mean pore diameter. Now the corrected tortuosity of the system attributed to an increase in path length due to obstruction by obstacles can be obtained by rearrangement from Eq. 11 using μ_{trans} as given by Eq. 15 (Fig. 6 *A*).

The "tortuosity" from Eq. 10 includes both Knudsen diffusion effects and corrected tortuosity as defined in Eq. 11. If the dominant contribution to the tortuosity is Knudsen diffusion only, then $\mu_{eff} \approx \varphi\mu_{trans}$ and the tortuosity defined by Eq. 10 would be given by

$$\tau_k = \frac{\phi\mu_0}{\phi\mu_{trans}} = \frac{\beta_0\sigma_p + \nu}{\beta_0\sigma_p} \quad (16)$$

and Eq. 16 would completely describe the data. Fig. 6 *B* shows the curve for Eq. 16 compared with the simulation results. This curve does not account for tortuosity at particle diameters less than 400 μm as can be seen by comparison to the simulation results.

Test for anomalous diffusion

Anomalous diffusion is found over longer distances as one approaches the percolation transition (Saxton, 1994), which for the current application would correspond to a sphere-packing fraction near the value of porosity below which bacterial migration is not possible. Because of the manner in which our porous media is constructed, and in view of the finite size of the bacteria, it is not clear a priori how close the porosity we have chosen is to the percolation transition. A plot of $\log(\Omega/t)$ as a function of $\log t$, where Ω is the mean-square displacement, has been shown by Saxton (1994) to provide a reliable indication of anomalous diffusion. For normal diffusion, the slope of the line is zero, whereas for the anomalous case the slope approaches $2/d - 1$, where d is an anomalous diffusion exponent specified by the anomalous diffusion equation (Saxton, 1994).

Fig. 7 is a plot of $\log(\Omega/t)$ as a function of $\log t$ for the simulations of Fig. 3. In Fig. 7 the slope of each line is effectively zero, which indicates that random motility in the model media is not related to anomalous diffusion. One important consequence of this is that the model can be translated mathematically into differential form for use by environmental engineers for predicting and designing bioremediation strategies in the field without recourse to anomalous diffusion theory.

The lack of evidence for anomalous diffusion is likely to be because a random dispersion of spheres has a porosity far from the percolation point. Roberts and Schwartz (1985) consider a range of media constructed from spherical grains and report percolation porosity's between 0.029 and 0.0055. This range of values is significantly different from the porosity of 0.37 found for the experimental system and used in

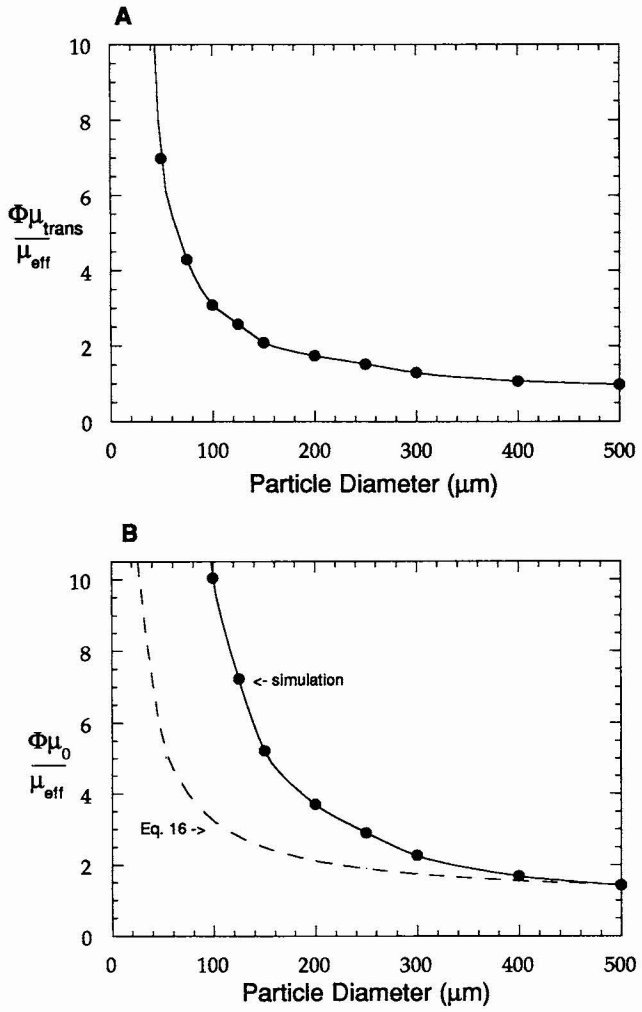

FIGURE 6 (*A*) Simulation results for $\beta_0 = 0.5$ using Eq. 11. (*B*) Comparison of Eq. 16 with the simulation results for $\beta_0 = 0.5$.

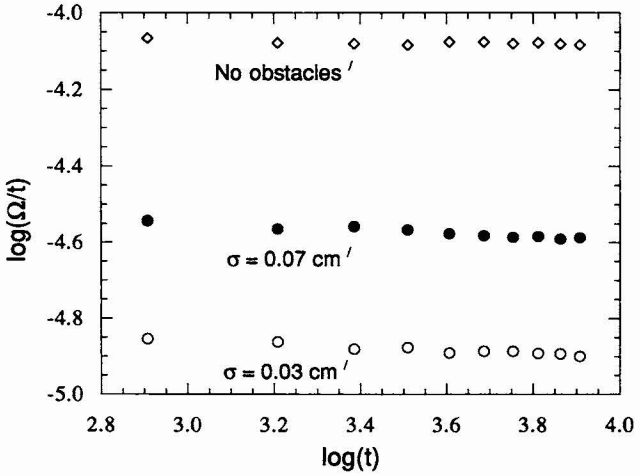

FIGURE 7 A test for anomalous diffusion by graphing $\log(\Omega/t)$ against $\log t$ using the data presented in Fig. 3.

the model. Excluded volume considerations arising from the finite size of the bacteria apparently do not decrease the effective porosity to values approaching the percolation transition.

CONCLUSIONS

Experimental data from bacterial migration in saturated sand columns indicate that as obstacle size decreases the tortuosity associated with the porous matrix increases. For smaller obstacle diameters, this effect is significant. Random walk simulations show that this effect is primarily due to the geometry of the media. The dominant aspects of this are the ratio of mean free path of the bacteria to pore diameter and the increase in the number of run segments needed (and thus the greater time required) to cover the same radial distance.

Other factors currently not taken into account in the simulations may play an important role in improving the agreement with experiment. One likely such mechanism is surface interactions between bacteria and obstacles that can be expected to reduce the random motility coefficient and, thus, increase the tortuosity. The extent of this effect depends on the number of bacteria-obstacle collisions. This in turn will depend on the obstacle surface area to pore volume ratio. We are currently designing experiments to measure surface interaction effects on the motility of the bacteria. Once completed the actual mechanisms of these interactions will be incorporated into the current algorithm.

When designing bioremediation strategies, it will be important to account for the soil geometry, which is shown here to have a significant influence on the random motility of bacteria. However, the algorithm developed here can also be used in the future to test models for surface interactions and their effect on bacterial motility. For example, a better understanding is needed of the role of bacteria-obstacle surface interactions and the importance of chemotaxis for bacterial motility in porous media. The importance of these contributions can be tested by comparing simulations of behavior with future experiments.

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