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NUMERICAL SOLUTION OF TRANSPORT EQUATIONS FOR BACTERIAL CHEMOTAXIS: EFFECT OF DISCRETIZATION OF DIRECTIONAL MOTION∗

BENJAMIN J. BROSILOW†, ROSEANNE M. FORD‡, STEN SARMAN§, AND PETER T. CUMMINGS¶

Abstract. A mathematical model proposed by Alt [J. Math. Biol., 9 (1980), pp. 147–177] to describe chemotactic bacterial migration is studied, and solutions to this model are compared to solutions of a simpler model proposed by Rivero et al. [Chemical Engineering Science, 44 (1989), pp. 2881–2897]. It is found that a discretized version of Alt’s model produces solutions similar to the continuous model, even at very coarse discretization. The relationship between the discretized Alt model and the model of Rivero et al. is elucidated, and it is found that a slightly modified version of the Rivero et al. model produces solutions similar to those of the Alt model for systems with one- and two-dimensional attractant gradients, suggesting that the simple and easy-to-use Rivero et al. model (after slight modification) is adequate for modeling bacterial behavior within the parameter ranges investigated. A preliminary investigation of the use of the lattice Boltzmann method for the study of bacterial migration is reported.

Key words. chemotaxis, bacteria, transport phenomena, balance equations, lattice Boltzmann method

AMS subject classifications. 60J60, 82A70, 92A08

1. Introduction. The directed migration of bacterial populations in response to chemical gradients is known as chemotaxis. For many years, there has been interest in the development of transport equations to quantitatively describe such chemotactic bacterial migration [22, 2, 4, 19, 20, 23, 24, 30]. The relationships between these various models for bacterial motion and the cell balance equations resulting from the models are reviewed by Ford and Cummings [11]. In the present paper, we present an investigation of one such bacterial transport equation proposed by Alt [2].

The recent interest in cell balance equations such as the Alt equation has been generated, in part, by the usefulness that a quantitative description of bacterial migration could potentially play within the context of optimizing bioremediation of hazardous wastes and providing quantitative prediction of the spread of bacteria released into the environment [16, 7, 32]. The Alt equation is of particular interest due to its direct relationship to fundamental bacterial behavior and the relatively few assumptions and idealizations about bacterial behavior that go into the equation’s derivation.

2. The cell balance equation. The Alt equation describes the motion of bacteria as though each individual bacterium were a random walker tracing out a piecewise linear path with a speed dependent on both time and position. Each linear portion of the bacterial motion is called a run, while each point at which the bacterium changes its direction of motion is called a tumble. The probability density that a bacterium

∗Received by the editors February 27, 1995; accepted for publication (in revised form) September 11, 1995. This research was supported by a grant from the IBM Environmental Research Program.
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tumbles at a given instant is called the \textit{tumble frequency} of the bacterium. In its most
general form, the equation derived by Alt [2] allows the tumble frequency to be a
function of time, velocity, position, and the amount of time that has elapsed since the
given bacterium’s last tumble. In the present paper we consider only a special case
of Alt’s equation where bacterial running speed is assumed to be constant, and the
tumble frequency is allowed to depend only on position, running direction, and time.
With these simplifications, the Alt equation reduces to

\begin{equation}
\frac{\partial n(X, v, t)}{\partial t} = -v \cdot \nabla n(X, v, t) - \beta(X, v, t)n(X, v, t)
+ \int dv^* n(X, v^*, t)\beta(X, v^*, t)K(v|v^*).
\end{equation}

Here \(n(X, v, t)\) is the density of bacteria at position \(X\) moving with velocity \(v\) at time \(t\), and \(\beta(X, v, t)\) denotes the tumbling frequency of such bacteria. \(K(v|v^*)\) is the
probability density that a bacterium running in direction \(v^*\) before tumbling will run
in direction \(v\) after tumbling and is called the \textit{turn angle distribution} of the bacteria.
Note that the quantities \(X\) and \(v\) are vectors in three-dimensional space, and we
denote their vector status by using boldface lettering. Equation (1) is equivalent
to the cell balance equation derived by Stroock [30] as demonstrated by Ford and
Cummings [11]. Consequently, we shall refer to (1) as the Alt–Stroock equation in
this paper.

Equation (1) can be understood as a balance on the number of bacteria at position
\(X\) and time \(t\) that are moving in direction \(v\). The first term on the right-hand side of
(1) accounts for the accumulation of bacteria at position \(X\) due to bacterial motion
in direction \(v\). The second term accounts for the loss of bacteria with velocity \(v\) at
position \(X\) due to tumbling. The integral term accounts for the opposite process (i.e.,
the tumbling of bacteria moving in direction \(v^*\) which subsequently move in direction
\(v\)).

The particular form of the tumbling frequency \(\beta\) with which we will be concerned
in the present work was first proposed by Rivero et al. [25, 14], based on observations
made by Berg and Brown on wild and genetically altered strains of \textit{Escherichia coli} [8]:

\begin{equation}
\beta(X, v, t) = B \exp \left[ -\frac{\nu N_r K_d}{(K_d + a)^2} \left( \frac{\partial a}{\partial t} + v \cdot \nabla a \right) \right].
\end{equation}

Here \(a = a(X, t)\) is the concentration of a chemical species to which the bacteria
respond chemotactically, \(K_d\) is the dissociation constant between the chemical attractant
and its receptor on the cell surface, \(\nu N_r\) is a fitting factor proportional to the
average number of attractant receptors on the surface of a single bacterium, and \(B\) is
the basal tumbling frequency, equal to the frequency at which the bacteria tumble in
the absence of both spatial and temporal attractant gradients. We note that in (2)
the dependence of \(\beta\) on position and time comes about via the dependence of \(a(X, t)\)
on position and time, and the dependence of \(\beta\) on the bacterial running direction is
incorporated via the term \(v \cdot \nabla a(X, t)\) in the exponent.

Equations (1) and (2) are based on a number of idealizations of bacterial behavior.
The validity of these idealizations is reviewed in detail elsewhere [8, 11, 14]. Generally,
the model accurately describes many important aspects of the behavior exhibited by
bacteria such as \textit{E. coli} and is one of the more detailed models for bacterial motion
studied to date. However, there are still a number of important aspects of bacterial
behavior that have not been included in the model, and we mention four of these.
aspects here: (1) The model assumes that bacteria “run” in straight paths. In fact, *E. coli* have been observed to exhibit rotational drift during their runs, causing their direction of motion at the end of a run to differ from that at the beginning of a run by an angle $\theta \sim 0.5\sqrt{t}$, where $t$ is the time duration of the run in seconds. Thus *E. coli*, with an average tumbling frequency of about 1 per second (in the absence of an attractant gradient), will end a run swimming about 30° from the direction in which the run was started [4]. By ignoring the rotational drift of the bacteria, we expect the model to overestimate the strength of the chemotactic response of a bacterial population to a given gradient. This is because the rotational drift adds a random, diffusive component to an otherwise directed motion of the bacteria. (2) The model assumes that “tumbles” are instantaneous or, equivalently, that the “tumbles” are negligibly short in comparison to run times. For *E. coli*, tumbles actually take an average of one tenth of a second, while run times are of the order of 1–10 sec (depending on the orientation of the run with respect to an attractant gradient) [5]. By ignoring the finite tumbling time, we expect the model to slightly overestimate the speed with which the bacteria respond to a given attractant gradient, since in fact the bacteria spend a finite time sitting in place while they tumble, and this time is unaccounted for in the model. (3) The model assumes that bacterial running speed is constant and uniform throughout the entire bacterial population. *E. coli* populations have been observed to have a distribution of average running speeds for individual members of the population, with a variance of about 25% of the mean running speed [5]. (4) The model assumes that bacterial tumbling is a Poisson process and that all the bacteria in a given population have the same expected tumbling frequency. In fact, individual *E. coli* do seem to tumble with an exponential distribution of run times, but the expected tumbling frequency exhibits some variation from individual to individual [5]. By ignoring the variance in running speeds and expected tumbling frequencies of the bacterial population, we expect that the Alt–Stroock equation will predict somewhat sharper bacterial concentration profiles than would be achieved by actual bacteria, since the variance in the behavior of the bacteria will result in the spreading of their final positions.

In this paper, we will concentrate our attention on several aspects of the numerical solution of (1). For the case of one-dimensional attractant gradients, this equation has been solved by using a finite-element technique by Frymier, Ford, and Cummings [15]. In this paper, we show that the numerical solution of the equation is remarkably accurate despite very coarse discretizations in $\theta$, the angle between the velocity vector of a moving bacterium, and the gradient direction. We also consider the reduction of the equation to essentially a one-dimensional equation similar to that considered by Rivero et al. [25], which we shall refer to as the RTBL equation. We investigate the difference between the discretized version of (1) and the RTBL equation, showing that after slight modification the RTBL equation can provide a good approximation to (1) in systems with one-dimensional attractant gradients. We investigate the solution of (1) in systems with two-dimensional attractant gradients and demonstrate that after slight modification the RTBL equation can again provide a good approximation to (1). Finally, the surprising accuracy of the coarsely discretized version of (1) led us to investigate whether a lattice Boltzmann approach might represent a viable method of solution for the full three-dimensional version of the equation.

3. Discretization of the cell balance equation. We begin our investigation of the cell balance equation, (1), by defining coordinate systems in which to express the position and direction vectors $\textbf{X}$ and $\textbf{v}$. As shown in Fig. 1, we have chosen to
Fig. 1. The relative orientation of the coordinate systems for defining the bacterial velocity vector \( \mathbf{v} = (\theta, \phi) \) and the bacterial position vector \( \mathbf{X} = (x, y, z) \).

Define the direction vector \( \mathbf{v} \) in terms of two scalars, \( \theta \) and \( \phi \). Note that since the bacterial running speed \( v = |\mathbf{v}| \) is assumed to be constant, we do not need to specify a third scalar in order to define a particular \( \mathbf{v} \). Figure 1 also shows the orientation of the \( x-, y-, \) and \( z- \) axes which we use to define the bacterial position vector \( \mathbf{X} = (x, y, z) \).

With \( \mathbf{v} \) defined as in Fig. 1, we can formally discretize (1) in velocity space by defining two sets of angles \( \{\theta_i\} \) and \( \{\phi_j\} \) such that \( 0 \leq \theta_i < \theta_{i+1} \leq \pi \) and \( 0 \leq \phi_j < \phi_{j+1} \leq 2\pi \). We can then define \( n_{i,j}(\mathbf{X}, t) \) as the density of bacteria at position \( \mathbf{X} \) with velocity in the interval \( (i,j) \),

\[
n_{i,j}(\mathbf{X}, t) = \int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} n(\mathbf{X}, \mathbf{v}, t) d\phi d\theta,
\]

and \( \beta_{i,j} \) as the expected tumbling frequency for a uniform distribution of bacteria in the velocity interval \( (i,j) \),

\[
\beta_{i,j}(\mathbf{X}, t) = \frac{\int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} \beta(\mathbf{X}, \mathbf{v}, t) d\phi d\theta}{\int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} d\phi d\theta}.
\]

If we assume that within each interval \( n(v, \mathbf{X}, t) \) and \( \beta(v, \mathbf{X}, t) \) are constant, then we can integrate (1) over interval \( (i,j) \) to get

\[
\frac{\partial n_{i,j}}{\partial t} = -\mathbf{v}_{i,j} \cdot \nabla n_{i,j} - \beta_{i,j} n_{i,j} + \sum_{k=1}^{N} \sum_{l=1}^{M} n_{k,l,i} \beta_{k,l,i} K_{k,l,i,j},
\]

where \( N \) and \( M \) are the number of intervals in the \( \theta \) and \( \phi \) directions, respectively, and

\[
\mathbf{v}_{i,j} = \frac{\int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} \mathbf{v} d\phi d\theta}{\int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} d\phi d\theta},
\]

\[
K_{k,l,i,j} = \frac{\int_{\theta_{k-1}}^{\theta_k} \sin \theta^* \int_{\phi_{l-1}}^{\phi_l} \int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} K(\theta, \phi; \theta^*, \phi^*) d\phi d\theta d\phi^* d\theta^*}{\int_{\theta_{k-1}}^{\theta_k} \sin \theta^* \int_{\phi_{l-1}}^{\phi_l} d\phi^* d\theta^*}.
\]
In other words, \( v_{i,j} \) is the expected velocity for a uniform distribution of bacteria in the velocity interval \((i, j)\), and \( K_{k,l,i,j} \) is the conditional probability that a bacterium will start a run in velocity interval \((i, j)\), given that the bacterium tumbled after running with a uniformly distributed velocity in interval \((k, l)\). We can evaluate (6) further by noting from Fig. 1 that the \( x\), \( y\), and \( z\)-components of \( v \) are \( v(x) = v \sin \theta \cos \phi \), \( v(y) = v \sin \theta \sin \phi \), and \( v(z) = v \cos \theta \), respectively. Therefore, the three components of \( v_{i,j} \) are

\[
(8) \quad v_{(x)ij} = \frac{v(\sin \phi_j - \sin \phi_{j-1})(\theta_{i} - \theta_{i-1} + \cos \theta_{i-1} \sin \theta_{i} - \cos \theta_{i} \sin \theta_{i})}{2(\phi_j - \phi_{j-1})(\cos \theta_{i-1} - \cos \theta_{i})},
\]

\[
(9) \quad v_{(y)ij} = \frac{v(\cos \phi_j - \cos \phi_{j-1})(\theta_{i} - \theta_{i-1} + \cos \theta_{i-1} \sin \theta_{i} - \cos \theta_{i} \sin \theta_{i})}{2(\phi_j - \phi_{j-1})(\cos \theta_{i-1} - \cos \theta_{i})},
\]

\[
(10) \quad v_{(z)ij} = \frac{v(\sin^2 \theta_i - \sin^2 \theta_{i-1})}{2(\cos \theta_{i-1} - \cos \theta_{i})}.
\]

We drop the \( j \) subscript from \( v_{(z)ij} \) since \( v_{(z)} \) does not depend on \( \phi \).

The assumption that \( n(v, X, t) \) and \( \beta(v, X, t) \) are constant within each interval will in general be exactly true only in the limit of infinitesimal intervals; hence (5) is equivalent to (1) only in this limit. However, we will show in the remainder of this work that there exist many practical situations in which very few intervals are needed for (5) to have nearly the same solution as (1).

### 4. Cell balance equation for one-dimensional attractant gradients.

In this section we consider the effect on (1) and (5) of restricting the tumbling frequency \( \beta \) to be a function of \( z \), \( \theta \), and \( t \) only. Restricting \( \beta \) in this way is equivalent to restricting the attractant gradient \( \nabla a \) to have zero \( x \)- and \( y \)-components, as can be seen from (2). Integrating the discretized Alt–Stroock equation (5) with respect to \( x \) and \( y \) over the entire cross-sectional area of the system gives

\[
(11) \quad \frac{\partial c_{i,j}}{\partial t} = -v_{(z)ij} \frac{\partial c_{i,j}}{\partial z} - \beta_i c_{i,j} + \sum_{k=1}^{N} \sum_{l=1}^{M} \beta_k c_k \sum_{l=1}^{M} K_{k,l,i,j},
\]

where \( c_{i,j}(z,t) = \int \int n_{i,j}(X,t)dx \, dy \), and \( \beta_i = \beta_{i,j} \) for all \( j \) since we assume in this section that \( \beta \) is not a function of \( \phi \); hence from (4), \( \beta_{i,j} \) is not a function of \( j \). We next sum (11) over all \( j \) (or, equivalently, integrate over all \( \phi \)) to get

\[
(12) \quad \frac{\partial c_i}{\partial t} = -v_{(z)i} \frac{\partial c_i}{\partial z} - \beta_i c_i + \sum_{k=1}^{N} \beta_k \sum_{l=1}^{M} c_{k,l} \sum_{j=1}^{M} K_{k,l,i,j},
\]

where \( c_i = \sum_{j=1}^{M} c_{i,j} \).

Since the presence of an attractant does not alter the turn angle distribution for small bacteria such as \( E. \ calor\) [8, 25], we will consider \( K(v|v^\ast) \) to be a function of the angle between \( v \) and \( v^\ast \) only (and not a function of the absolute direction of either of the vectors). For such \( K \) it is possible to simplify (12) further, since in this case \( K(v|v^\ast) \) is a function of the absolute value of the difference \(|\phi - \phi^\ast|\) but not a function of either angle separately, and so it follows that \( K_{k,l,i,j} \) is a function of \( k \),
and |j - l| only. Thus \( \sum_{j=1}^{M} K_{k,l,i,j} \) is a function of \( k \) and \( i \) only, which makes it possible to remove this summation from inside the summation over \( l \) in (12):

\[
\frac{\partial c_i}{\partial t} = -v(z) \frac{\partial c_i}{\partial z} - \beta c_i + \sum_{k=1}^{N} \beta_k c_k \sum_{j=1}^{M} K_{k,l,i,j},
\]

where we have arbitrarily chosen to evaluate \( K_{k,l,i,j} \) at \( l = 1 \), since \( \sum_{j=1}^{M} K_{k,l,i,j} \) does not vary with \( l \).

Thus (13) is equivalent to (5) in the case where \( \beta = \beta(z, \theta, t) \) (i.e., one-dimensional gradient) and \( K(v|v^*) \) is a function of only the angle between \( v \) and \( v^* \), and (5) is in turn equivalent to the Alt–Stroock equation (1) in the limit of infinitesimal velocity–space intervals. To investigate how many velocity intervals are actually necessary to reasonably approximate the continuum Alt–Stroock equation (1) using (13), we have integrated (13) numerically at various levels of velocity–space discretization for the stopped flow diffusion chamber (SFDC) assay of Ford et al. [13], and our results are plotted in Fig. 2. In the SFDC geometry, described briefly in Appendix A, the bacterial concentration \( c_i(z, t) \) is initially (at \( t = 0 \)) uniform for all \( i \) and \( z \), while the attractant concentration \( a(z, t) \) is taken to be a decaying step function:

\[
a(z, t) = \frac{a_0}{2} \left[ 1 + \text{erf} \left( \frac{z}{\sqrt{4D_a(t + \tau)}} \right) \right].
\]

Here \( D_a \) is the diffusion coefficient of the attractant, \( a_0 \) is the height of the step change in attractant concentration, and \( \tau \) is an offset time determined by the particular

**FIG. 2.** Bacterial profiles at \( t = 4 \) minutes in the SFDC geometry as predicted by various models. The solid curve shows the solution to the discretized Alt–Stroock equation (13) in the continuum limit, which is equivalent to the solution to the Alt–Stroock equation (1). The dashed curve shows the solution to (13) when only two intervals are used in the \( \theta \)-direction. The dashed curve is also the solution to the two-interval steady-flux model (22), (23), (24) and the modified RTBL model (22), (27), (28). The dotted curve is the solution to the unmodified RTBL model (22), (25), (26). The vertical dotted line at \( z = 0 \) shows the position of the initial step change in attractant concentration, with an initial concentration of \( a = 0 \) to the left of the line and \( a = 0.2 \text{ mM} \) to the right of the line. (Note that this step change was allowed to decay for \( \tau = 15 \) sec before the numerical solution was begun, as described by (14).)
experimental conditions (as described in Appendix A and [13, 28]). We have used the values given in Table 1 for the attractant and bacterial properties in all the numerical solutions presented in this work. These constants are appropriate for describing the response of *E. coli* bacteria to the attractant α-methylaspartate [15, 29]. For the turn angle distribution $K(\psi^*)$, we used a form derived from the data of Berg and Brown [5] for *E. coli*. The details of this function are described in Appendix B of this paper, but generally this turn angle distribution is biased toward small turn angles (so that the bacteria exhibit persistence in their direction of motion).

We note that in (14) the attractant profile is not coupled to the bacterial profile. This is a consequence of the fact that *E. coli* do not metabolize α-methylaspartate. In the general case where the bacteria in question do metabolize the attractant, (14) should be replaced by a diffusion equation with appropriate bacterial concentration-dependent terms for attractant consumption. This diffusion equation would need to be integrated simultaneously with (13). Note that there is no significant computational advantage in decoupling the attractant concentration profile from the bacterial concentration profile. We have used the decoupled attractant profile of (14) simply because this profile is appropriate for the *E. coli*/α-methylaspartate system, which has been the subject of experimental studies [5, 6, 15, 26, 27].

The solid line in Fig. 2 shows the solution to (13) for the SFDC geometry (14) at $t = 4$ minutes, where the bacterial concentration was everywhere set initially to 1 (i.e., $1 = \sum_{i=1}^{N} c_i(z, t = 0)$), the attractant step height $a_0$ was 0.2 mM, and the offset time $\tau$ was 15 sec. Note that the solution to (13) using 50 intervals in the $\theta$ direction differed from the solutions using 20, 10, or 5 intervals by less than $4 \times 10^{-3}$ units at all points, rendering the solutions at these various discretizations indistinguishable from each other on the scale on which they are plotted in the figure. Thus we conclude that in this case only 5 intervals in the $\theta$ direction are necessary for the velocity and space-discretized Alt–Stroock equation (13) to have essentially the same solution as the continuum equation (1). The dashed line of Fig. 2 shows the solution to (13) with only two intervals in the $\theta$ direction, and even this proves to be a fair approximation to the continuum Alt–Stroock equation. Note that when we refer here to a solution of (13), we are referring to the distribution of the measurable quantity $c = \Sigma c_i$ and not the distribution of the individual $c_i$.

The solutions presented in Figs. 2, 4, and 6 were generated by integrating the appropriate equations in time using explicit first-order differencing with a time-step $\Delta t = 0.001$ sec. A second-order differencing scheme was used along the $z$-axis, with $\Delta z = 1/400$ cm. All systems were 1 cm in length, with no flux boundary conditions used at the endpoints. The solutions did not change when $\Delta t$ or $\Delta z$ were decreased or when the system length was increased. When dividing the velocity space into intervals, we chose $\{\theta_i\}$ according to the formula $\theta_i = \arccos(1 - 2i/N)$, where $N$ is the number of intervals in the $\theta$ direction. Choosing $\{\theta_i\}$ in this way ensured that

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
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</thead>
<tbody>
<tr>
<td>$D_a$</td>
<td>$6.9 \times 10^{-6}$ cm$^2$/sec</td>
<td>[13, 12]</td>
</tr>
<tr>
<td>$v$</td>
<td>0.0022 cm/sec</td>
<td>[18]</td>
</tr>
<tr>
<td>$B$</td>
<td>0.17/sec</td>
<td>[14]</td>
</tr>
<tr>
<td>$K_d$</td>
<td>0.08 mM</td>
<td>[17]</td>
</tr>
<tr>
<td>$\nu/N_r$</td>
<td>72 sec</td>
<td>[14]</td>
</tr>
</tbody>
</table>
each interval had equal area in velocity space. (Note that the area of an interval in velocity space is \( \int_{\theta_{i-1}}^{\theta_i} \sin \theta \int_{\phi_{j-1}}^{\phi_j} d\phi d\theta \).) The values of \( K_{k,l,i,j} \) were calculated using 16-point Gaussian quadrature of the integrals in (7).

5. RTBL-like approximations to the cell balance equation with one-dimensional attractant gradients. In their comparative study of cell balance equations, Ford and Cummings [11] provided a partial analysis of the relationship between the RTBL one-dimensional cell balance equation [25] and the balance equation obtained from (1) by integrating out the two spatial dimensions in which there is symmetry. Ford and Cummings found that the symmetrized version of (1) did not reduce to the RTBL equation and that there were some obvious discrepancies in the role of the velocity in the two equations. In this section, we investigate the relationship between the two equations in greater detail, demonstrating that the discretized version of (1) for a one-dimensional gradient is similar in form to the RTBL equation when just two intervals are used for \( \theta \).

To explicitly write (13) for the case of two velocity–space intervals, we define \( \theta_0 = 0, \theta_1 = \pi/2 \), and \( \theta_2 = \pi \) (and \( \phi_0 = -\pi, \phi_1 = \pi \)). Then, for each interval, (13) can be rearranged to give

\[
\frac{\partial c_1}{\partial t} = -v(z)_{11} \frac{\partial c_1}{\partial z} - P_1 c_1 + P_2 c_2,
\]

\[
\frac{\partial c_2}{\partial t} = -v(z)_{22} \frac{\partial c_2}{\partial z} + P_1 c_1 - P_2 c_2,
\]

where \( P_1 = \beta_1 K_{1,1,1,1} \) and \( P_2 = \beta_2 K_{2,1,1,1} \). If we call the region \( \theta_0 < \theta < \theta_1 \) velocity interval 1 and \( \theta_1 < \theta < \theta_2 \) velocity interval 2, then, in other words, \( P_1 \) is the probability that at a given instant a bacterium running with velocity in interval 1 will tumble and then begin a new run with velocity in interval 2, and \( P_2 \) is the probability that at a given instant a bacterium running with velocity in interval 2 will tumble and then begin a new run with velocity in interval 1. From (10) we can see that \( v(z)_{11} = v/2 \) while \( v(z)_{22} = -v/2 \).

We note that (15) and (16) have the same form as the equations of Rivero et al. [25] for their one-dimensional RTBL model, although our constants \( v(z)_{11} \) and \( P_1 \) differ somewhat from those of Rivero and co-workers. We proceed to follow the analysis of Rivero et al. applying it to (15) and (16). First we define the bacterial flux in the \( z \)-direction as \( J_z(z, t) = v(z)_{11} c_1 + v(z)_{22} c_2 \) and the total bacterial concentration as \( c(z, t) = c_1 + c_2 \). Then adding (15) and (16) gives

\[
\frac{\partial c}{\partial t} = -\frac{\partial J_z}{\partial z},
\]

while subtracting (15) from (16) and multiplying the resulting equation by \( v/2 \) give

\[
\frac{\partial J_z}{\partial t} = -\left(\frac{v}{2}\right)^2 \frac{\partial c}{\partial z} - \frac{v}{2} (P_1 - P_2) c - (P_1 + P_2) J_z.
\]

If we approximate that \( \partial J_z/\partial t \approx 0 \), then we can rearrange the above equation to get

\[
J_z = -\mu \frac{\partial c}{\partial z} + V_c c.
\]
with
\[ \mu = \frac{v^2}{4(P_1 + P_2)} \]
and
\[ V_c = v(P_1 - P_2)/(2(P_1 + P_2)), \]
Substituting (19) into (17) gives
\[ \frac{\partial c}{\partial t} = \frac{\partial}{\partial z} \left( \mu \frac{\partial c}{\partial z} - V_c c \right). \]
\(\mu\) is referred to as the “random motility coefficient” of the bacteria, and \(V_c\) is called the “chemotactic velocity.” These names come from the observation that (22) has the form of a one-dimensional diffusion equation with bulk flow, where \(\mu(z, t)\) corresponds to the diffusion coefficient and \(V_c(z, t)\) corresponds to the bulk flow rate. Evaluating \(P_i = \beta_i K_{1,1,2,1}\) using (4) and (2) and plugging the result into the expressions for \(\mu\) and \(V_c\), (20) and (21), give
\[ \mu = \frac{v^2}{8BK_{1,1,2,1}} \frac{\alpha v \frac{\partial a}{\partial z}}{\sinh(\alpha v \frac{\partial a}{\partial z})}, \]
\[ V_c = \frac{v}{2} \tanh \left[ \alpha \frac{v \frac{\partial a}{\partial z}}{2} \right], \]
where \(\alpha = \nu N_v K_d / (K_d + a)^2\). We will call the approximation to the Alt–Stroock equation given by (22), (23), and (24) the “two-interval steady-flux model,” since (22), (23), and (24) are equivalent to the discretized Alt–Stroock equation (13) with two velocity–space intervals, with the additional assumption of steady bacterial flux \(\partial J_z/\partial t \approx 0\).

The formulas for \(\mu\) and \(V_c\) for the two-interval steady-flux model differ from those derived by Rivero et al. [25] for the RTBL model:
\[ \mu_{RTBL} = \frac{v^2}{2BK_{1,1,2,1}} \exp \left[ \alpha \frac{\partial a}{\partial t} \right] \frac{\partial a}{\partial z}, \]
\[ V_{cRTBL} = v \tanh \left[ \alpha \frac{v \frac{\partial a}{\partial z}}{2} \right]. \]

We can derive formulas for \(\mu\) and \(V_c\) that are more similar in form to those of the RTBL model if, instead of using (4) to evaluate \(\beta_i\), we simply let \(\beta_i = \beta(z, \theta', t)\) for some \(\theta'\) in the interval \(i\). If, for example, we chose \(\theta' = \pi/3\) in interval 1 and \(\theta' = 2\pi/3\) in interval 2, we would get from using (2), (20), and (21)
\[ \mu' = \frac{v^2}{8BK_{1,1,2,1}} \exp \left[ \alpha \frac{\partial a}{\partial t} \right] \frac{\partial a}{\partial z}, \]
\[ V'_c = \frac{v}{2} \tanh \left[ \alpha \frac{v \frac{\partial a}{\partial z}}{2} \right]. \]
These two equations are simply the RTBL model equations with $v$ replaced everywhere by $v/2$, as was first suggested by Ford and Cummings [11]. We will refer to (27) and (28) as the “modified RTBL model.” This model is, like the two-interval steady-flux model, equivalent to the discretized Alt–Stroock equation (13) with two velocity–space intervals, with the additional assumption of steady bacterial flux $\partial J_z/\partial t \approx 0$. The form of the modified RTBL model differs from the form of the two-interval steady-flux model due to different approximations used in each model for the average value of the tumbling frequency $\bar{\beta}$ in each interval. Figure 3 shows a comparison between the forms of $\mu$ and $V_c$ for the various models. The two-interval steady-flux model and modified RTBL model are virtually identical, while the RTBL model differs significantly from the other two. Figure 2 demonstrates that the RTBL model gives a poor approximation to the Alt–Stroock equation, while the two-interval steady-flux and modified RTBL models give results virtually identical to a two-interval approximation to the Alt–Stroock equation (implying that $\partial J/\partial t = 0$ is a good approximation in this case).

The models developed in this section rest on two approximations: (a) that two intervals in velocity space are sufficient for the discretized Alt–Stroock equation (13) to approximate the continuum Alt–Stroock equation and (b) that $\partial J_z/\partial t \approx 0$. The relatively good agreement between the two-interval steady-flux model and the continuum Alt–Stroock equation solution shown in Fig. 2 indicates that these approximations are reasonable under the typical experimental conditions simulated there. However, both of these approximations become poorer as the attractant gradient $\nabla a$ becomes larger. This is demonstrated in Fig. 4, where we have modeled the same conditions as in Fig. 2, except that the step change in attractant concentration was 100 times as large, the offset time $\tau$ was half as long, and the system was simulated for only 10
sec. These extreme conditions were chosen because they expose the bacteria to a very large and sharp attractant gradient throughout the entire numerical integration. Under these conditions, the two-interval steady-flux model significantly overshoots the solution to the discretized Alt–Stroock equation (13) with two intervals, in addition to completely missing the secondary peak in bacterial concentration at $z \approx -0.04$ cm, implying that $\partial J_z/\partial t$ is not small in this case. Also, the solution to the discretized Alt–Stroock equation (13) using two intervals significantly overshoots the solution to the continuum equation, implying that more than two intervals are necessary for (13) to approximate the continuum equation (1). For the solution to the discretized Alt–Stroock equation to differ from the continuum solution everywhere by less than $4 \times 10^{-3}$ units in Fig. 4, about 15 $\theta$-intervals are needed.

In Fig. 5 we have replotted the data of Fig. 4 using the same scale as that in Fig. 2 and also have plotted the solutions to the various models at $t = 4$ minutes under the high-attractant gradient conditions of Fig. 4. From this figure we can see that the deviations between the models shown in Fig. 4 are relatively short-lived, and the models produce similar solutions as time increases and the high-attractant gradient decays via diffusion. Thus we conclude that even in the relatively extreme conditions simulated in Figs. 4 and 5, the coarsely discretized Alt–Stroock equation and the RTBL-like models give a fair approximation to the continuum Alt–Stroock equation solution after the attractant gradient is allowed to decay for a short time.

To ensure that the secondary peak shown by the solid curve of Fig. 4 was not an artifact of the second-order differencing scheme used along the $z$-axis, the integration
Fig. 5. Bacterial profiles at $t = 4$ minutes (large loops) and $t = 10$ sec (small loops) in the SFDC geometry as predicted by various models. The conditions are the same as those in Fig. 2, except that the step change in attractant concentration is 100 times as large, and the relaxation time $\tau = 7$ sec is half as long. The solid curves are solutions to (13) in the continuum limit or, equivalently, the solutions to the continuum Alt–Sirock equation (1). The dashed curves are solutions to (13) with two intervals in the $\theta$-direction. The dotted curves are solutions to the modified RTBL model.

of (13) in the continuum limit was repeated, using a first-order differencing scheme along the $z$-axis, with results identical to those shown in Fig. 4. (The explicit first order integration used 20 $\theta$-intervals, 10,000 $z$-intervals/cm, and a time step of 0.001 sec.)

6. Saturation of the attractant sensing mechanism. A comparison of Figs. 2 and 5 reveals that the increased attractant gradient of Fig. 5 produces no increase in the chemotactic response of the bacteria and that the region in which the chemotactic response occurs is shifted down-gradient in Fig. 5. These observations can be explained in terms of the inability of the modeled bacteria to sense the higher attractant concentrations present near the step change in attractant concentration in Fig. 5. Physiologically, the failure of bacteria to sense an attractant gradient occurs when the attractant concentration is sufficiently high that all the attractant receptors on the surface of the bacteria remain bonded to attractant molecules nearly all the time. The bacteria then have no way of sensing further increases in attractant concentration. This "saturation" of the attractant sensing mechanism is incorporated in the models via the factor $1/(K_d + a)^2$ in the exponential of (2). This factor causes the bacterial tumbling frequency $\beta$ to rapidly approach $B$, the tumbling frequency in the absence of a gradient, as the attractant concentration $a$ increases beyond a value on the order of $K_d$. Hence Fig. 5 shows a chemotactic response mainly in the region $z < 0$ where the attractant concentration is below saturation.

7. The effect of persistence in the bacterial random walk. The numerical results presented in Figs. 2 and 4 were obtained by using a form for $K(v\cdot v^*)$ which was biased toward small turn angles, giving the bacterial random walk a persistence
in the direction of motion (appropriate for the simulation of E. coli). To see the effect that such a directional persistence has on the bacterial concentration profile, we performed numerical integrations on systems identical to those of Figs. 2 and 4, except that different forms of $K(v|v^*)$ were used. Figure 6 shows solutions for the case of a uniform $K(v|v^*) = 1/(4\pi)$ and for a form of $K(v|v^*)$ which is a "mirror image" of the form used to generate the data of Figs. 2 and 4. The details of this "mirror image" form of $K$ are presented in Appendix B, but generally this $K$ was biased toward large turn angles in the same way as the $K$ of Figs. 2 and 4 was biased toward small turn angles.

The results plotted in Fig. 6 show that as the persistence of the bacterial random walk increases, the bacterial concentration peak becomes shorter and wider and the concentration trough becomes shallower and wider. Also, as the persistence increases, the overall bacterial concentration in the high attractant concentration region decreases, meaning that persistence in the bacterial random walk decreases the chemotactic response of the bacteria. This trend can be understood in terms of the RTBL-like models, (22)–(28). These models divide the behavior of the bacteria into two parts: a purely diffusive behavior, characterized by $\mu$, and a chemotactic behavior, characterized by $V_c$. While the chemotactic behavior tends to establish regions of high bacterial concentration where there is high attractant concentration, the diffusive behavior tends to smooth such bacterial concentration peaks toward a uniform concentration profile. One can see that for any of the RTBL-like models, $V_c$ is unaffected
by the form of $K$ and hence the persistence of the bacterial random walk, while $\mu$ is inversely proportional to the probability $K_{1,1,2,1}$ that a bacterium will change its direction by tumbling with a large turn angle. Hence increasing persistence in the bacterial random walk increases the diffusive behavior of the bacteria, which counteracts the chemotactic motion of the bacteria. Indeed, the increased width of the peaks and troughs in the bacterial concentration profiles of Fig. 6 for the persistent bacterial random walks attests to the increased diffusivity associated with these bacteria.

We note that in all the RTBL-like models, the factor $K_{1,1,2,1}$ appears only as a product with the basal tumbling frequency, $BK_{1,1,2,1}$. Thus increasing $K_{1,1,2,1}$ (or equivalently, increasing the turn angle bias toward large turn angles) has the same effect as increasing the basal tumbling frequency $B$. This can be understood by considering that for an unbiased random walker in three-dimensional space (i.e., Brownian motion) the diffusion constant is given by $D = \nu \ell / 3$ [4], where $\nu$ is the particle velocity and $\ell$ is the mean distance traveled between changes in the random walker's direction of motion. For bacteria, $\ell$ would correspond to the ratio $\nu / (BK_{1,1,2,1})$ (with $\nu$ the swimming speed of the bacteria), since a bacterium must both tumble and choose a large turn angle in order to appreciably change its direction of motion. Thus the bacterial diffusivity $\mu$ depends on $K$ and $B$ only as the product $BK_{1,1,2,1}$.

While the RTBL-like models are able to describe the trends shown in Fig. 6, one would expect them to fail to accurately describe what occurs when the bacterial turn angle distribution is sharply peaked at turn angles near $\pi$ (so that the bacteria nearly reverse direction after every tumble, i.e., a very nonpersistence random walk). In this case, one would still expect bacteria to show a strong chemotactic response after long exposures to a given gradient, but at shorter exposure times the response should not be as strong since some bacteria will become "trapped" moving perpendicular to the gradient. This occurs because turn angles near $\pi$ keep the bacterial motion restricted to approximately a straight line. RTBL-like models cannot describe this phenomenon since they are based on the assumption of steady flux $\partial J_x / \partial t \approx 0$, and bacteria with turn angle distributions strongly peaked near $\pi$ require long times to reach their equilibrium velocity distribution, so $\partial J_x / \partial t \neq 0$ at short times for such bacteria.

Note that for some bacterial species the turn angle distribution is quite different from that measured by Berg and Brown [5] for wild-type E. coli. For example, Duffy, Cummings, and Ford [10] report the turn angle distribution for Pseudomonas putida, which is found to be bimodal with peaks near 0 and $\pi$ corresponding to the predominantly backward and forward motion of this bacterial species. Thus, consideration of unusual turn angle distributions, such as that considered above, may be physiologically relevant as well as mathematically useful as a probe of the accuracy of numerical approximations.

8. The cell balance equation for two-dimensional attractant gradients. We have solved the general discretized Alt–Stroock equation (5) on an effectively infinite system where the bacterial concentration profile is initially (at $t = 0$) a Gaussian,

$$c(x, y, t) = \frac{4 - \pi}{4\pi \sigma^2_t} \exp \left[ -\frac{4 - \pi}{4\sigma^2_t} (x^2 + y^2) \right],$$

and the attractant profile is a decaying Gaussian of height $a_0$ at time $t = 0$,

$$a(x, y, t) = \frac{a_0 \tau}{t + \tau} \exp \left[ -\frac{1}{4D_a(t + \tau)} ((x - x_0)^2 + (y - y_0)^2) \right].$$
Fig. 7. Contours of the bacterial concentration profile for an initial Gaussian distribution of bacteria centered on the solid black dot, responding to an attractant concentration profile diffusing from an initial Gaussian distribution centered on the small open circle. The initial attractant Gaussian was of width 0.05 cm and height 0.2 mK, and the initial bacterial Gaussian was of width 0.05 cm and height \((4 - \pi)/(4\pi\sigma_\beta^2) = 27.3\) units. A box surrounding the contours of 0.5-cm length on each side is drawn to provide a length scale. The solid lines are contours of the solution to the discretized Alt–Stroock equation (5) in the continuum limit (15 θ intervals and 15 φ intervals). The dashed lines are contours of the solution to (5) with 4 velocity–space intervals, as described in the text. The dotted lines (virtually on top of the dashed lines) are contours of the solution to the two-dimensional modified RTBL model. Contours are shown at (a) \(t = 2\) minutes and (b) \(t = 4\) minutes. In both cases, outer contours are for a bacterial concentration of 1, and inner contours are for a bacterial concentration of 10.

Here \(\sigma_\beta\) is the width (that is, standard deviation in radial direction) of the initial bacterial Gaussian distribution, and \(\sqrt{4\pi D_\beta} \sigma_\beta\) is the width of the initial attractant Gaussian distribution. We chose \(\sigma_\beta = \sqrt{4\pi D_\beta} \sigma_\beta = 0.05\) cm for our numerical solutions. The attractant profile was centered at \(x_0 = 0.15\) cm and \(y_0 = 0.15\) cm from the bacterial peak so that the total distance between the initial bacterial and attractant peaks was 0.212 cm. As in the previous numerical solutions, the attractant and bacterial properties were characterized using the constants of Table 1, appropriate for describing the response of the bacteria \(E.\) coli to the attractant \(\alpha\)-methylaspartate. This geometry can be thought of as corresponding to a laboratory experiment in which a petri dish containing a solution of buffer mixed with a small amount of agar is inoculated with bacteria at time \(t = 0\). Simultaneously, a small droplet of an attractant is placed near the inoculation point, and the spread of bacteria away from the inoculation point is observed. Results of the numerical solution are shown in Fig. 7.

We also performed calculations using a “two-dimensional modified RTBL” model characterized by the equation

\[
\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial c}{\partial x} - V_{cx} c \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial c}{\partial y} - V_{cy} c \right),
\]
with $\mu_x$ and $\mu_y$ defined by (27) with $z$ replaced everywhere by $x$ or $y$, respectively, and $V_{cx}$ and $V_{cy}$ defined by (28) with $z$ again replaced by $x$ or $y$, respectively. This model is thus just the one-dimensional modified RTBL model applied in the $x$- and $y$-directions independently. We would not expect this model to accurately represent the Alt–Stroock equation in the presence of a strong gradient, since the model does not account for the correlation between the bacterial motion in the $x$- and $y$-directions. Nonetheless, Fig. 7 shows that this model approximates the continuum Alt–Stroock equation solution at least as well as the discretized Alt–Stroock equation (5) with 4 velocity intervals, which does account for the correlation between the bacterial motion along each axis. (The 4 intervals in this discretization were defined by $\phi_0 = -\pi/4$, $\phi_1 = \pi/4$, $\phi_2 = 3\pi/4$, $\phi_3 = 5\pi/4$, and $\phi_4 = 7\pi/4$, and $\theta_0 = 0$, $\theta_1 = \pi$.)

In order to test the two-dimensional modified RTBL model under more stringent circumstances, we also performed numerical solutions on systems similar to those of Fig. 2, except that instead of starting with a uniform bacterial concentration, we began with a Gaussian bacterial distribution centered on the step change in attractant concentration (see Fig. 8). For this system one would expect that the bacterial motion along the $x$- and $y$-directions would be strongly correlated near the step change in attractant concentration, since near this step change the bacteria strongly bias motion toward the positive $x$-direction (up the attractant gradient) at the expense of their motion in the $y$-direction. Thus one would expect that the gradient in the $x$-direction would strongly decrease the $y$-direction diffusivity $\mu_y$ near the step change. But apparently this effect can be ignored, since the two-dimensional modified RTBL

![Contour plots](image)

**Fig. 8.** Contours of the bacterial concentration profile for an initial Gaussian distribution of bacteria centered on the solid black dot. The bacteria are responding to a diffusing step change attractant gradient. The attractant was initially at concentration 0.2 mM to the right of the dotted line and 0 mM to the left of the line, as described by (14), with an offset time $\tau = 15$ sec. The shape of the initial bacterial Gaussian was the same as in Fig. 7, and the meaning of the various contours is the same as in that figure. Also as in Fig. 7, (a) shows contours for $t = 2$ minutes, and (b) shows contours for $t = 4$ minutes.
model again approximates the continuum Alt–Strook equation at least as well as the four-interval solution to the discretized Alt–Strook equation (5).

The solutions presented in Figs. 7 and 8 were generated by integrating the appropriate equations in time using explicit first-order differencing with a time-step \( \Delta t = 0.05 \) sec. A second-order differencing scheme was used along the \( x \)- and \( y \)-directions, with \( \Delta x = \Delta y = 1/100 \) cm. The solid curves were generated using a velocity–space discretization of 15 \( \theta \)-intervals and 15 \( \phi \)-intervals. When dividing the velocity space into intervals, we chose \( \{\theta_i\} \) according to the formula \( \theta_i = \text{Arc cos}(1 - 2i/N) \), where \( N \) is the number of intervals in the \( \theta \) direction as discussed in §4. Values of \( \{\phi_j\} \) were chosen according to the formula \( \phi_j = 2\pi(j - 0.5)/M \), where \( M \) is the number of intervals in the \( \phi \)-direction. Choosing \( \phi_j \) in this way caused the first \( \phi \)-interval to be symmetric about the \( x \)-axis (see Fig. 1).

9. Lattice Boltzmann method. In contrast to numerically solving the Alt–Strook cell balance equation, (1), to predict bacterial density profiles, a quite distinct approach is to perform simulations of the dynamics of individual cells and infer population behavior by averaging over their motion, much as one can obtain bulk thermophysical properties by statistical averaging over individual molecular motions in molecular-level simulations of fluids [1]. One such brute-force Monte Carlo simulation methodology, which we termed cellular dynamics (CD), was developed in which the motion of many (typically \( 10^5 \)) individual bacteria in the SFDC (see Appendix A) was simulated, using experimentally determined mean run lengths and turn angle distributions [14]. The advantage of CD is that it can be used in any situation, including bacterial migration in a model porous medium [10] and is not tied to a particularly simple form of the chemoattractant gradient or any particular geometry; its weakness is that, like any \( N \)-body simulation technique for the calculation of collective properties, the noise level in the simulations is \( O(N^{-1/2}) \) so that high-accuracy predictions come at prodigious computational cost.

For the high-symmetry case of bacteria responding to a one-dimensional chemoattractant gradient, as in the SFDC, the full numerical solution to (1) can be obtained with little difficulty, as shown in §4 above and in [15]. The advantage of the numerical solution is that it is essentially noise-free; its weakness is that it is difficult to extend to three-dimensional systems, particularly for the complex geometry associated with bacterial migration in porous media characteristic of saturated soil.

In the preceding sections, one conclusion that emerges is that the full numerical solution of the Alt–Strook equation for the SFDC can be approximated reasonably well by a numerical solution in which the angular motion of the bacteria is divided into only two elements (i.e., \( 0 \leq \theta < \pi/2 \) and \( \pi/2 \leq \theta < \pi \)). This suggests that the density profiles resulting from a chemotactic response may be insensitive to some of the details of the angular motion of the bacteria. This observation further suggests that a simulation methodology that exploits this insensitivity might provide an efficient mechanism for the simulation of bacterial migration in complex, three-dimensional systems. Lattice gas and lattice Boltzmann models are simulation methodologies which are specifically designed to exploit the insensitivity of large-scale phenomena to the directional details of the underlying microscopic phenomena and are therefore appropriate methods to consider for simulating bacterial migration. During the last decade lattice gas models have been applied to solve partial differential equations (PDEs), particularly the Navier–Stokes equation for flow through porous media. At first stochastic methods were devised [9] in which a lattice gas was simulated in order to solve the PDE. The drawback of these lattice gas methods is that long simulations
must be performed in order to minimize the statistical noise. It was later shown that the statistical noise could be overcome by solving the lattice Boltzmann equation [31, 3]. In the remainder of this section, we describe the successful development of a lattice Boltzmann method (LBM) for modeling the migration of chemotactic bacteria and compare our results with full numerical solutions of the same balance equation and experimental data.

We begin by writing the Alt–Stroock equation, (1), in a slightly different and more obviously symmetrical form,

\[
\frac{\partial n(X, \hat{s}, t)}{\partial t} = -v\hat{s} \cdot \nabla [n(X, \hat{s}, t)]
\]

\[+ \int d\hat{s}^* p(\hat{s}^*, \hat{s}, X, t)n(X, \hat{s}^*, t) - \int d\hat{s}^* p(\hat{s}, \hat{s}^*, X, t)n(X, \hat{s}, t),\]

where \(n(X, \hat{s}, t)\) is the number of bacteria at position \(X\) per unit volume per unit solid angle swimming in the \(\hat{s}\) direction at time \(t\) and \(p(\hat{s}, \hat{s}^*, X, t)\) is the probability per unit time per unit solid angle that a bacterium swimming in the direction \(\hat{s}\) tumbles and subsequently moves in the direction \(\hat{s}^*\). In the notation of (1), \(v = v\hat{s}\) and \(p(\hat{s}, \hat{s}^*, X, t) = \beta(X, v, t)K(v^*|v)\). Equation (32) was derived in this form by Stroock [30] prior to the work of Alt [2, 23]. The similarity of (32) to the Boltzmann equation suggests that an LBM may be an appropriate and efficient way to solve (32). We constrain the bacteria to swim in discrete lattice directions (in our case, the six directions \((\pm x, \pm y, \pm z)\) associated with the three-dimensional cubic lattice) and allow bacteria to change from one discrete direction to another only after a tumble. When the directions are discretized, (32) becomes

\[
\frac{\partial n_\alpha(X, t)}{\partial t} = -v\hat{s}_\alpha \cdot \nabla [n_\alpha(X, t)] + \sum_{\beta=1}^{L} T_{\alpha\beta}(X, t)n_\beta(X, t),
\]

where

\[
T_{\alpha\beta}(X, t) \equiv p_{\beta\alpha}(X, t) - \delta_{\alpha\beta} \sum_{\gamma=1}^{L} p_{\alpha\gamma}(X, t),
\]

\(n_\alpha(X, t)\) is the number of particles moving in the \(\hat{s}_\alpha\) direction, \(p_{\alpha\beta}(X, t)\) is the probability per unit time that a bacterium tumbles and changes direction from lattice direction \(\hat{s}_\alpha\) to lattice direction \(\hat{s}_\beta\), and \(L\) is the number of directions in which a particle can travel. This equation is formally the same as the lattice Boltzmann equation [31, 3]. The transition matrix \(T_{\alpha\beta}(X, t)\) plays the same role as the collision operator. Note, however, that there are no collisions between the bacteria. The change of direction occurs because the bacterium itself decides to tumble. Discretizing (33) with respect to time and space and replacing the derivatives with finite differences yields

\[
n_\alpha(X + \Delta x_\alpha, t + \Delta t) = \left(1 - v \frac{\Delta t}{\Delta x}\right)n_\alpha(X + \Delta x_\alpha, t) + \left(v \frac{\Delta t}{\Delta x}\right)n_\alpha(X, t) + \sum_{\beta=1}^{L} T_{\alpha\beta}(X, t)n_\beta(X, t)\Delta t,
\]
where $\Delta x_\alpha$ is the vector displacement between adjacent lattice points in the $\alpha$ direction. The application of (35) can be regarded as the repeated execution of two steps. The first step is the collision step corresponding to tumbling in bacterial migration. In this step the collision operator redistributes particle density between the different directions. In the second step, the propagation step, the particle density travels to the next lattice point in the direction of its velocity. When the lattice Boltzmann equation is used to solve the Navier–Stokes equation, all the particle density travels to neighboring lattice points ($v\Delta t/\Delta x = 1$). For our application to bacterial migration the factor $(1 - v\Delta t/\Delta x)$ means that this fraction of the bacterial density stays at the lattice point and only a fraction $v\Delta t/\Delta x$ continues to neighboring lattice points.

In this section, we use as the model for $p(\hat{s}, \hat{s}^*, X, t)$ the functional form

$$p(\hat{s}, \hat{s}^*, X, t) = \min \left[ B \exp \left[ \frac{-\nu N_r K_d}{[K_d + a(X, t)]^2} (\hat{s} \cdot \nabla a(X, t)) \right] K(\hat{s}^*|\hat{s}), BK(\hat{s}^*|\hat{s}) \right].$$

(36)

This differs slightly from the expression used in previous sections, (2), since (36) embodies the assumption that when a bacterium is experiencing a decreasing attractant concentration (equivalent spatially to moving down an attractant gradient or away from an attractant source) it reverts to the basal tumbling frequency $B$ exhibited in the absence of an attractant in accordance with some experimental evidence for E. coli [8, 12, 13, 14]. The motivation for not considering return to basal frequency in the previous sections was to permit direct comparison with the model used by Rivero et al. [25] in which (2) was assumed.

In our lattice model, we have only six different directions and thus a discrete turn angle distribution. We have chosen it in such a way that $\langle \cos \theta \rangle$ and $\langle \cos^2 \theta \rangle$ are the same as in the continuous distribution. In order to test our lattice Boltzmann algorithm, we have chosen to solve (32) for the SFDC using the same parameters as Frymier, Ford, and Cummings [15], which are given in Table 1. Following Frymier, Ford, and Cummings, we also select a small 0.8-cm $\times$ 0.04-cm $\times$ 0.04-cm region at the center of the SFDC to model. We use 400 lattice points in the $z$-direction and 20 points in the $x$- and $y$-directions, giving a lattice spacing, $\Delta x$, of 0.002cm. The time-step, $\Delta t$, is 0.02 sec, so $v\Delta t/\Delta x = 0.022$. The bacterial density reported is

$$c(z, t) = \iiint d\hat{s} dx dy n(X, \hat{s}, t).$$

In Fig. 9 we compare bacterial density profiles obtained with the full finite element method (FEM) solution of Frymier, Ford, and Cummings [15] and the LBM at 2, 4, and 6 minutes after the start of the SFDC experiment. The initial attractant concentration on the right-hand side of the chamber is $a_0 = 0.2$ mM. For comparison purposes, the parameter $\tau$ in (14) was set to $\tau = 0$ as in Frymier, Ford, and Cummings [15]. Despite the approximation introduced by constraining the motion to a simple cubic lattice, the LBM profile virtually coincides with the FEM profile. We find similarly good agreement between LBM and FEM for $\nu N_r$ as large as $2 \times 10^3$ sec, corresponding to the largest measured value of this quantity [21] found in bacteria cultured in nutrient-limited conditions.

In Fig. 10, we present a comparison between the LBM solution and experimental data for E. coli responding to $\alpha$-methyIaspartate in the SFDC [29]. The parameters used in the model are $\nu N_r = 78.5$ sec, $a_0 = 0.01$ mM, $D_a = 7.1 \times 10^{-6}$ cm$^2$/sec,
Fig. 9. The dimensionless bacterial density, $b/b_0$, as a function of the $z$-coordinate at three times (2, 4, and 6 minutes) after the start of the SFDC experiment. The dashed curves depict the density obtained by the LBM, and the solid curves depict the density obtained from the full solution to (32).

Fig. 10. The dimensionless bacterial density, $b/b_0$, as a function of the $z$-coordinate at three times (1, 2, and 4 minutes) after the start of the SFDC experiment. The full curves depict the density obtained by the LBM. The symbols are experimental data for E. coli responding to $\alpha$-methylaspartate in the SFDC [29].
\[ K_d = 0.125 \text{ mM}, \; v = 22 \mu m/\text{sec}, \; \text{and} \; B = 2.87 \text{ sec}^{-1}. \] 

The large value of \( B \) is required to be consistent with the experimentally measured random motility of \( \mu_0 = 8.8 \times 10^{-7} \text{ cm}^2/\text{sec} \) for the strain of \( E. coli \) used by Strauss et al. [29]. To account for the fact that experimentally it is impossible to begin with a perfect step function in attractant concentration, the time delay parameter in (14) is set to \( \tau = 10 \text{ sec} \) so that the initial attractant profile is a slightly relaxed version of a step function. The comparison indicates that the model is quite accurate in predicting the bacterial density profiles measured experimentally.

### 10. Conclusions

We have investigated the effect of velocity–space discretization on the Alt–Stroock equation and found that very coarse discretizations of the Alt–Stroock equation produce results similar to the continuum solution. Further, the less detailed and easier to solve model of Rivero et al. can be interpreted as a discretized Alt–Stroock model with two velocity–space intervals plus the additional assumption of steady bacterial flux \( \partial J/\partial t = 0 \). Replacing the bacterial velocity \( v \) in the RTBL model with half the actual velocity \( v/2 \) is equivalent to choosing nodes near the center of each velocity interval in the discretized Alt–Stroock equation; hence this substitution results in solutions for the RTBL model which more closely follow the solutions of the continuum Alt–Stroock equation.

The effects of directional persistence in bacterial random walks were briefly investigated, and it was found that persistence decreases the rate at which bacteria migrate toward an attractant source. The modified RTBL model proved useful for describing qualitative trends associated with the persistence, demonstrating that persistent random walks produce a larger diffusive term \( \mu \) than nonpersistent walks, while the chemotactic term \( V_c \) is unaffected by the degree of persistence.

In the presence of two-dimensional attractant gradients, a modified RTBL model applied independently in the \( x \)- and \( y \)-directions produces solutions similar to the Alt–Stroock equation. We find this result surprising, because intuitively one expects there to be a correlation between the bacterial velocities in the \( x \)- and \( y \)-directions, which is ignored in the two-dimensional modified RTBL model of (31). Apparently this correlation is sufficiently weak that it can be ignored without substantially affecting the solution of the model.

Finally, we presented the solution to the cell balance equation for the SFDC by a lattice Boltzmann model method and validated its accuracy by comparing to a finite-element solution of the same equation for a highly symmetric case. In less regular geometries, such as porous media, which are of great practical importance, the numerical problem becomes intractable for finite-element or finite-difference methods. The only feasible method previously available to us was the CD method, for which very long simulation runs are required to prevail over the statistical noise. The LBM method does not suffer from any of these disadvantages. We will report on its application to bacterial migration in saturated porous media in a future publication.

### Appendix A. The SFDC Assay

An experimental assay frequently used to measure the random motility \( \mu_0 \) and the chemotactic sensitivity coefficient \( \chi_0 = \nu N_c v^2 \) is the SFDC assay developed by Ford and co-workers [13, 12] (Fig. 11). Two glass microscope slides form the walls of the 4-cm \( \times \) 2-cm \( \times \) 0.2-cm chamber. The triangular packed beds at the top and bottom help dissipate the momentum of the incoming fluid and evenly distribute flow across the width of the chamber. Two bacterial suspensions differing only in the concentration of an attractant are initially contacted by impinging flow driven by a syringe pump. The impinging flow pattern creates a step change in the attractant concentration at the center of the chamber.
while maintaining a uniform distribution of bacteria throughout the chamber. Note that fluid exits the chamber through ports located on each side of the center of the chamber. The experiment begins \((t = 0)\) when the impinging flow is halted, and the attractant begins diffusing into the attractant-free half of the chamber while the bacteria migrate toward the region with higher attractant concentration. For short times, the temporal and spatial dependence of the attractant concentration is given by the solution of the one-dimensional diffusion equation with a step function as the initial condition and boundary conditions \(a(z, t) = a_0, z \to \infty\), and \(a(z, t) = 0, z \to -\infty\):

\[
(37) \quad a(z, t) = \frac{a_0}{2} \left[ 1 + \text{erf} \left( \frac{z}{\sqrt{4D(t + \tau)}} \right) \right],
\]

where \(D\) is the diffusion coefficient of the attractant. The offset time \(\tau\) is necessary in (37) since a finite impinging flow rate does not produce a perfect step function of attractant (i.e., \(\tau \to 0\) only in the limit of infinitely fast impinging flow) [13, 28].

**Appendix B. The turn angle distribution for *E. coli.*** The turn angle distribution \(K(v|v^*)\) of (1) is defined by

\[
(38) \quad K(v|v^*) = \frac{f(\psi)}{2\pi \sin(\psi)},
\]
where $\psi$ is the angle between the vectors $\mathbf{v}$ and $\mathbf{v}^*$ and $f(\psi)$ is the probability density that a given tumble will result in a turn angle of magnitude $\psi$. If we express each of the velocity vectors $\mathbf{v}$ and $\mathbf{v}^*$ in terms of the pair of angles $(\theta, \phi)$ and $(\theta^*, \phi^*)$, respectively, as indicated in Fig. 1, then we can express $\psi$ as

$$\psi = \text{Arc cos}[\sin \theta \sin \theta^* (\sin \phi \sin \phi^* + \cos \phi \cos \phi^*) + \cos \theta \cos \theta^*].$$

(39)

The functional form of $f(\psi)$ has been calculated for *E. coli* by Frymier, Ford, and Cummings [14] by fitting a sixth-order polynomial to the data in Berg and Brown (Fig. 3 of [5]) as follows:

$$f(\psi) = c_1(\pi - \psi)^6 + c_2(\pi - \psi)^5 + c_3(\pi - \psi)^4 + c_4(\pi - \psi)^3 + c_5(\pi - \psi)^2 + c_6(\pi - \psi).$$

(40)

However, we observed that the fit found by Frymier, Ford, and Cummings [14] resulted in slightly negative values of $f(\psi)$ for $\psi > 3.08330168$. Thus we made use of (40) only in the range $0 \leq \psi \leq 3.08330168$ and define $f(\psi) = 0$ for $\psi > 3.08330168$. After renormalizing the fit of Frymier, Ford, and Cummings to account for the truncation of $f$ above $\psi = 3.08330168$, we find the following values for the constants in (40):

$c_1 = 2.00255E - 04$, $c_2 = 1.88105E - 02$, $c_3 = -1.29520E - 02$, $c_4 = 8.02005E - 03$, $c_5 = 1.33743E - 04$, and $c_6 = -2.80659E - 05$. Equation (40) with the aforesaid constants is plotted in Fig. 12.

![Graph](image.png)

**Fig. 12.** The turn angle distribution $f(\psi)$ described in Appendix B. $f(\psi)$ is the probability density that a given tumble by a bacterium will result in a turn angle $\psi$. Note that an unbiased turn angle distribution is represented by $f(\psi) = \sin(\psi)/2$.

In §6 we have made use of a “mirror image” form of $K$. This $K$ is defined by

$$K(\mathbf{v} | \mathbf{v}^*) = \frac{g(\psi)}{2\pi \sin(\psi)},$$

(41)

where $g(\psi) = f(\pi - \psi)$.
Acknowledgments. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the IBM Corporation. The authors thank Paul Frymier for his assistance in preparing several of the figures and Dr. John A. Somers of Shell Research, Amsterdam, for helpful suggestions concerning lattice gas automata and lattice Boltzmann methods.

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