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Application of Stochastic Computer Simulation to a Solution of a Nonlinear Fokker–Planck Equation Governing Bacteria Chemotaxis

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A stochastic computer simulation technique has been used to solve a one-dimensional time-dependent Fokker–Planck (F–P) equation governing space-time distribution of bacteria in a substrate (food) gradient. Because of consumption of the substrate by the bacteria the F–P equation becomes nonlinear due to coupling of the distribution with the self-generated substrate gradient. The simulation is efficient and numerically accurate for generating transient solutions. We are able not only to produce a transient solution displaying approach to the steady state solitary wave solution known from an analytical result of Keller and Segal but also to show an interesting dependence of the solitary wave propagation speed on the concentration dependence of the substrate consumption rate.

KEY WORDS: Computer simulation; chemotaxis; stochastic computer simulation.

1. INTRODUCTION

Chemotaxis refers to a manifestation by certain strains of bacteria of having the ability to sense the presence of chemical gradients of nutrients or of toxic agents. Chemotaxis in bacteria was already discovered by biologists Engelmann[1] and Pfeffer[2] in the late nineteenth century but much more quantitative work was done on the model bacteria *Escherichia coli* in the late sixties by Adler and coworkers.[3,4] Adler specifically studied

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chemotaxis of *E. coli* to oxygen (also called aerotaxis), amino acids, and sugars and was able to identify specific "chemo-receptor proteins" located in the cell membrane for each of these "chemoeffectors." *E. coli* was used as a model sensory system because of its simplicity, the ease of isolating the receptor proteins, and its ease of generic manipulation.[5]

The simplest demonstration of the phonomenon of chemotaxis is to inject suitable numbers of motile *E. coli* into the bottom of a tube containing oxygen-saturated motility buffer solution. A sharp band of the bacteria is soon formed and the band migrates slowly upward because the bacteria collectively seek a certain optimum oxygen concentration within a traveling oxygen gradient created by their metabolism. If the buffer solution also contains nutrients such as serine or galactose then more than one band can form because the bacteria would follow both the oxygen gradient and, say, the serine gradient.[3] An example of such a band formation is given in Fig. 1.

A mathematical theory of this striking phenomenon of band formation and propagation was formulated by Keller and Segel[6] for the simplest case of one band. Consequences of the theory were quantitatively tested by

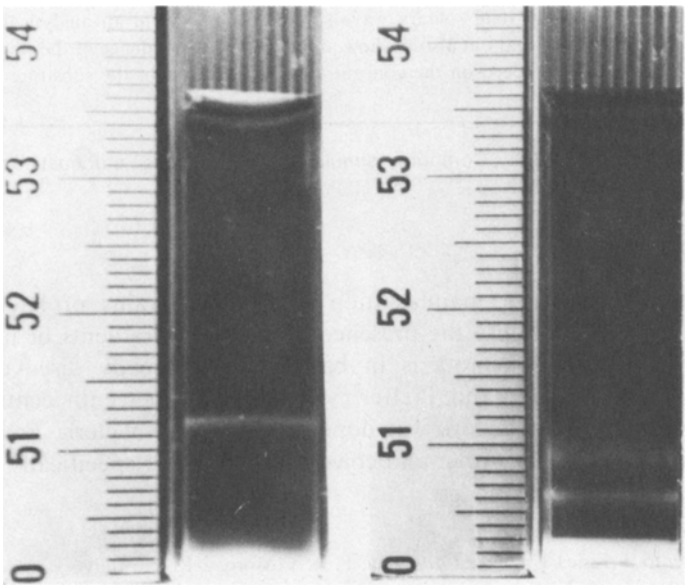

Fig. 1. Examples of *E. coli* chemotactic bands in motility buffer. When there is only the saturated oxygen as a substrate, there is one band. But when there is an additional substrate such as serine present then it becomes possible to have two bands.

a light scattering experiment of Holz and Chen[7] recently. The Keller–Segel model of chemotaxis consists of a pair of coupled nonlinear Fokker–Planck equations involving the bacteria density $b(z,t)$ and the substrate concentration $c(z,t)$. Solution of these coupled equations generally requires a numerical procedure.[8,7]

A mathematically interesting case occurs in the Keller–Segel (K–S) model equations when the substrate concentration diffusion can be neglected. In this case the pair of nonlinear equations can be solved analytically in the traveling wave coordinate which respresents a steady state propagation of a bacterial band coupled to a substrate front. This solitary wave solution was tested experimentally by Holz and Chen[7] and they found it approximately valid in describing the band propagation in a liquid medium containing oxygen and serine. They pointed out, however, that diffusion of the substrate was not negligible and had to be taken into account in order to obtain a quantitative agreement between theory and experiment.

Nevertheless, this K–S model (with substrate diffusion neglected) is an elegant example of an analytically soluble model and is worth pursuing further. In this paper we describe a technique we are currently developing for numerical studies of the transition from the transient (band formation) to the steady state (band propagation) solution. With this method we are able first to show a transient solution which displays approach to the steady state solution of Keller and Segel; and next to show an interesting dependence of the band propagation speed on the substrate consumption rate of bacteria. This consumption rate was taken to be a constant in the K–S model but in actuality it should be a concentration dependent quantity.

In Section 2 we shall introduce briefly the K–S model, and its solution. In Section 3 we describe the technique of stochastic computer simulation for solution of nonlinear Fokker–Planck equations and then in Section 4 we present the results of the numerical study of the K–S model. We conclude in Section 5 with a summary and prospect of the future studies.

2. KELLER–SEGEL MODEL OF CHEMOTAXIS

Two variables of interest in the migrating band problem are $b(z,t)\,dz$, the number of bacteria per unit area between heights $(z, z + dz)$ at time t and $c(z,t)\,dz$, the number of substrate molecules per unit area between heights $(z, z + dz)$ at time t. The continuity equation expressing the conservation of the number of bacteria is then

$$\frac{\partial b}{\partial t} = -\frac{\partial}{\partial z}\left[-\mu\frac{\partial b}{\partial z} + v_c b\right] \tag{1}$$

The first term in the bracket on the right-hand side of the equation expresses the diffusion current in the z direction due to the random motion. This can be taken as a macroscopic manifestation of the microscopic random motion in the absence of chemotaxis. μ is the diffusion coefficient associated with the random walk and is called the "motility coefficient" in the context. The random walk is, however, biased toward the positive z direction. If the chemotaxis speed v_c were a constant, then Eq. (1) is nothing but a Fokker–Planck equation derivable from the Langevin equation of a particle in a constant external field.

The solution of Eq. (1) would then be a band propagating in the z direction with a constant speed v_c if initially formed. However, the situation is more complicated because of the fact that the chemotaxis is a result of the gradient sensing of the bacteria.[9] As a result, v_c is a function of the substrate concentration $c(z,t)$. The statement of this functional dependence is in essence the "law of chemotaxis." It can be formulated by putting

$$v_c(c) = \delta \frac{dF(c)}{dz} \tag{2}$$

where $F(c)$ is a nondimensional "sensitivity function" and δ the "chemotaxis coefficient" having a dimension of cm^2/sec. Keller and Segel[6] in their original paper took a specific form

$$F(c) = \ln\left(\frac{c}{c_{th}}\right) \tag{3}$$

where c_{th} may be thought of as the threshold concentration of the substrate below which the phenomenon of chemotaxis does not occur. Functional form of Eq. (3) was chosen because the logarithmic dependence of the sensitivity function on the concentration seemed related to the well-known Weber–Fechner law of sensing applicable for many biological situations.

With a choice of Eq. (3), Eq. (1) becomes

$$\frac{\partial b}{\partial t} = -\frac{\partial}{\partial z}\left[-\mu \frac{\partial b}{\partial z} + \frac{\delta}{c}\frac{\partial c}{\partial z} b\right] \tag{4}$$

Corresponding conservation equation for the substrate can be written down easily as

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial z}\left[-D\frac{\partial c}{\partial z}\right] - kb \tag{5}$$

where D is the diffusion coefficient of the substrate and k is the number of substrate molecules consumed per second per bacterium.

2.1. The Solitary Wave Equations

Experimenally[7] the bacteria form a sharp band after an initial transient period of several minutes. Then the band migrates at an approxi-

mately constant speed over a limited length of time (like 10 min). It is thus useful to make a transformation of the coordinates to a moving frame by setting

$$\xi = z - vt \tag{6}$$

$$\tau = t \tag{7}$$

where v is the migration speed of the band. Equations in the moving frame are obtained by replacing in Eqs. (4) and (5)

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} - v\frac{\partial}{\partial z}, \qquad \frac{\partial}{\partial z} \to \frac{\partial}{\partial \xi} \tag{8}$$

to get

$$\frac{\partial b}{\partial \tau} - v\frac{\partial b}{\partial \xi} = \mu\frac{\partial^2 b}{\partial \xi^2} - \frac{\partial}{\partial \xi}\left[\frac{\delta}{c}\frac{\partial c}{\partial \xi}b\right] \tag{9}$$

$$\frac{\partial c}{\partial \tau} - v\frac{\partial c}{\partial \xi} = D\frac{\partial^2 c}{\partial \xi^2} - kb \tag{10}$$

The experimental observation of a sharp band[7] suggests that we may put

$$b(\xi, \tau) = B(\xi) + b'(\xi, \tau) \tag{11}$$

$$c(\xi, \tau) = C(\xi) + c'(\xi, \lambda) \tag{12}$$

and over a limited period of time where the speed is constant, disregard the derivatives of b' and c' as compared to that of $B(\xi)$ and $C(\xi)$. Then

$$-v\frac{dB}{d\xi} = \mu\frac{d^2B}{d\xi^2} - \frac{d}{d\xi}\left[\frac{\delta}{C}\frac{dC}{d\xi}B\right] \tag{13}$$

$$-v\frac{dC}{d\xi} = D\frac{d^2C}{d\xi^2} - kB \tag{14}$$

2.2. Keller–Segel Limit

Equations (13) and (14) can be solved under the following boundary conditions: at

$$\xi = -L, \qquad C = \frac{dC}{d\xi} = 0 \tag{15}$$

$$\xi = L, \qquad C = C_0 \tag{16}$$

and at

$$\xi = \pm L \qquad B = \frac{dB}{d\xi} = 0 \tag{17}$$

where $\pm L$ refers to a large distance above and below the band. Then Eq.

(13) can be immediately integrated to give

$$B(z) = Re^{-x}\left[C(x)\right]^{\bar{\delta}} \tag{18}$$

where we introduce dimensionless variables $x = (v/\mu)\xi$, $\bar{\delta} = \delta/\mu$, and R is the constant of integration, which can be obtained by demanding that integration of $B(x)$ from $-L$ to L gives total number of bacteria in the band N.

Equation (18) indicates that the bacterial distribution peaks at x_0 where

$$\frac{d}{dx} \ln C(x)|_{x=x_0} = \frac{1}{\bar{\delta}} \tag{19}$$

Also by integrating both sides of Eq. (14) from $-L$ to $+L$, we get the speed of migration v:

$$v = \frac{kN}{AC_0} - \frac{D}{C_0} \frac{dC}{d\xi}\bigg|_L \tag{20}$$

where N stands for the total number of bacteria in the band and A the cross-sectional area of the tube. Substituting Eq. (18) into Eq. (14) and define dimensionless quantities

$$\bar{C}(x) = \frac{C(x)}{C_0} \tag{21}$$

$$\bar{D} = \frac{D}{\mu} \tag{22}$$

we can rewrite Eq. (14) as

$$\bar{D} \frac{d^2\bar{C}}{dx^2} + \frac{d\bar{C}}{dx} = Qe^{-x}\bar{C}(x)^{\bar{\delta}} \tag{23}$$

where

$$Q = \frac{k\mu}{v^2} C_0^{\bar{\delta}-1} R \tag{24}$$

Equation (23) in general can be solved numerically.[7] But in a special case when the motility coefficient μ is much larger than the substrate diffusion coefficient, or $\bar{D} \to 0$ which we shall call the Keller–Segel limit, it can be integrated simply to give an analytical solution

$$\bar{C}(x) = \left[1 + e^{-x}\right]^{-1/(\bar{\delta}+1)} \tag{25}$$

In this K–S limit we have from Eq. (20)

$$v = W = \frac{kN}{AC_0} \tag{26}$$

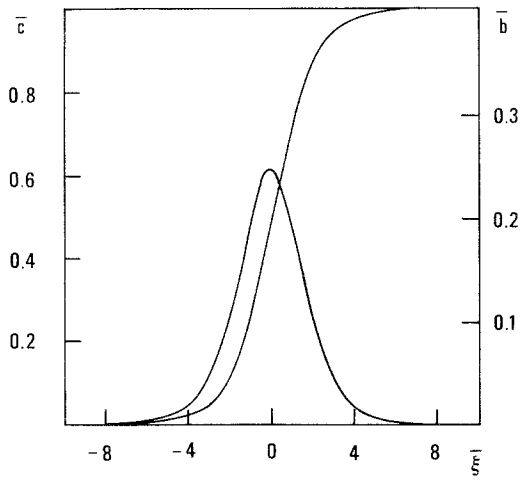

Fig. 2. An example of the Keller–Segel solution when $\bar{\delta} = 2$. The peak represents $B(\xi)$, the bacteria band.

where C_0 is the saturated substrate concentration in the medium in which bacteria is moving.

We shall normalize the bacterial density in such a way that

$$\bar{B}(x) = e^{-x}\left[\bar{C}(x)\right]^{\bar{\delta}}(\bar{\delta} - 1)^{-1} \tag{27}$$

This normalization corresponds to choosing the origin of the coordinate x_0 at the peak position of $\bar{B}(x)$. Figure 2 illustrates the K–S analytical solution for the case $\bar{\delta} = 2$.

2.3. Extension of K–S Solution

The K–S analytical solution Eqs. (25)–(27) was obtained under an assumption $k = \text{const}$. Physically this assumption is correct only when there is an abundance of the nutrient so that bacteria can consume at a constant rate. When the substrate is sufficiently depleted there will be a threshold concentration $\bar{C}_T$ below which the consumption rate k will be $\bar{C}$ dependent. We can write this dependence as

$$k(\bar{C}) = kf(\bar{C}) \tag{28}$$

Returning to Eq. (14) taking $D = 0$ we get

$$v\frac{d\bar{C}}{d\xi} = \frac{k}{C_0} f(\bar{C})B \tag{29}$$

It can be converted into

$$\int_0^1 \frac{d\bar{C}}{f(\bar{C})} = \frac{k}{C_0 v} \int_{-L}^{L} B(\xi)\, d\xi = \frac{kN}{C_0 A v}$$

Upon using relation Eq. (26) we get

$$\frac{W}{v} = \int_0^1 \frac{d\bar{C}}{f(\bar{C})} \tag{30}$$

which relates the band migration speed v to the K–S limiting value W given in Eq. (26).

We shall take a reasonable model

$$f(\bar{C}) = \begin{cases} \left(\bar{C}/\bar{C}_T\right)^{\alpha}, & \text{for } \bar{C} \leqslant \bar{C}_T \\ 1, & \text{for } \bar{C} \geqslant \bar{C}_T \end{cases} \tag{31}$$

This model says that the consumption rate is below the saturation value k below a threshold concentration $\bar{C}_T$ and it is equal to k above $\bar{C}_T$. Substituting Eq. (31) into Eq. (30) we obtain

$$\frac{v}{W} = \frac{1-\alpha}{1-\alpha\left(1-\bar{C}_T\right)} \tag{32}$$

Equation (32) shows that the band migration is possible only when $\alpha < 1.0$, and for these values of α the migration speed v is generally lower than the K–S value W. The dependence of v/W on $\bar{C}_T$ and α is depicted in Fig. 3.

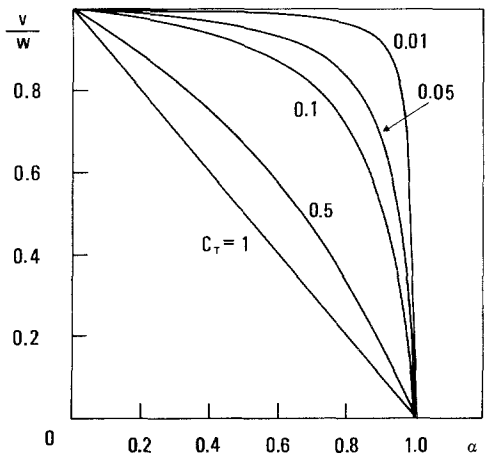

Fig. 3. v/W vs. α plots for different values of $\bar{C}_T$.

K–S equations can be solved analytically also for this model and we obtain a solution which is functionally the same as the K–S solution [Eq. (27)] for $x > x_T$ but is different for $x \leqslant x_T$. x_T is related to $\bar{C}_T$ by

$$x_T = \ln\left[\frac{\bar{C}_T^{\delta-1}}{1-\bar{C}_T^{\delta-1}}\right] \tag{33}$$

Physically, one can interpret this result as follows. In the K–S limit where the consumption rate k is a constant, bacteria form a well-defined band and the band migrates steadily. In a more realistic situation where the consumption rate is lower depending on the amount of nutrient present, having a definite threshold value $\bar{C}_T$, the tail part of the bacterial band is affected. The most interesting case corresponds to $\alpha = 1$ where Eq. (32) predicts $v = 0$. This means that if we initially set up a band, it will migrate only for a transient period of time and then eventually the bacteria will dissipate and the band will be lost. Physical reason for the dissipation is that the tail part of the bacterial band will gradually lag behind because of a lack of the substrate. There is experimental evidence that this is actually happening to many of *E. coli* bands we observe in the laboratory. In reality, all the *E. coli* bands one usually observes may well be transient bands since they only last a few hours at most. Therefore it is of great interest to investigate the transient solution of the K–S equation.

3. STOCHASTIC COMPUTER SIMULATION

Theoretically a relevant quantity to compute is: $P(z,t\,|\,z_0,0)\,dz$, which is a conditional probability that a bacterium will be at $(z, z+dz)$ at time t, if initially it is at z_0. $P(z,t\,|\,z_0,0)$ satisfies an initial condition

$$P(z,0\,|\,z_0,0) = \delta(z-z_0) \tag{34}$$

and boundary conditions

$$\left(\frac{\partial P}{\partial z}\right)_{z=0} = 0, \qquad P(\infty,t\,|\,z_0,0) = 0 \tag{35}$$

Since it is a conditional probability, one must have

$$b(z,t) = \int_0^\infty dz_0\, P(z,t\,|\,z_0,0)\, b(z_0,0) \tag{36}$$

This relation guarantees that $P(z,t\,|\,z_0,0)$ also satisfies the Fokker–Planck equation

$$\frac{\partial}{\partial t} P(z,t\,|\,z_0,0) = -\frac{\partial P}{\partial z}\left(-\mu\frac{\partial}{\partial z} + v_c P\right) \tag{37}$$

when $P(z,t\,|\,0,0)$ is known from solution of Eq. (37) the conservation of

bacteria Eq. (36) demands that for an initial distribution

$$b(z,0) = \frac{N}{A}\delta(z), \qquad b(z,t) = \frac{N}{A}P(z,t\,|\,0,0) \tag{38}$$

Instead of solving a nonlinear Eq. (37) numerically for the conditional probability $P(z,t\,|\,0,0)$, it is easier to transform it to an equivalent Langevin description which deals with the trajectory of bacteria. It is well known[10] that a stochastic differential equation for the position $z(t)$ is a bacterium which is equivalent to the Fokker–Planck equation (37) is

$$dz(t) = v_c dt + (2\mu)^{1/2} dW(t) \tag{39}$$

where $dW(t)$ is a stochastic Wiener process with properties

$$\langle dW(t)\rangle = 0 \tag{40}$$

$$\langle dW^2(t)\rangle = dt \tag{41}$$

$$\langle dW(t)\,dW(t')\rangle = \delta(t-t')\,dt\,dt' \tag{42}$$

As a consequence

$$v_c = \left\langle \frac{dz}{dt} \right\rangle \tag{43}$$

is the instantaneous velocity, or the instantaneous force (in this overdamped case) acting on an average bacterium which we called the chemotactic force. Thus it is useful to think of an effective potential $V(z)$ acting on each bacterium such that

$$v_c = -\frac{\partial V}{\partial z} \tag{44}$$

It is important to realize that v_c is not the drift velocity of the bacterial band. The drift velocity v is given by

$$v = \frac{d}{dt}\langle z\rangle \tag{45}$$

which we can calculate from a computer simulation.

If there is no finite potential barrier the bacteria will move in the range $(-\infty, \infty)$ on the z axis. In our case, the motion is bounded at $z = 0$ due to existence of the bottom of the cell. One has therefore to use the reflection principle of Désiré André (10) and introduce a reflecting barrier at the origin. This means that we use a new process which is equivalent $z(t)$ for $z \geqslant 0$ but to $-z(t)$ for $z > 0$.

We shall work in terms of scaled variables: $z = z_0\bar{z}$ and $t = t_0\bar{t}$ where $z_0 = \mu/v$ and $t_0 = \mu/v^2$. Then Eq. (39) can be written in terms of the scaled variables as

$$d\bar{z} = \bar{v}_c\,d\bar{t} + \sqrt{2}\,d\bar{W}(\bar{t}) \tag{46}$$

where

$$\bar{v}_c = \frac{v_c}{v} = \frac{\bar{\delta}}{\bar{C}} \frac{d\bar{C}}{d\bar{z}} \tag{47}$$

and v is the band migration speed.

In a stochastic computed simulation Eq. (46) is supplemented by a deterministic equation (K–S model)

$$\frac{\partial c}{\partial t} = -kf(C)b$$

which is written in a scaled form

$$\frac{\partial \bar{C}}{\partial \bar{t}} = -\bar{b}f(\bar{C}) \tag{48}$$

The scaling parameter for b is $b_0 = Nv^2/AW\mu$.

The computer simulation goes through the following steps:

(i) Choose a time and space interval $\Delta\bar{t}$ and $\Delta\bar{z}$ such that

$$\bar{t}_n = n\Delta\bar{t}, \qquad \bar{z}_i = i\Delta\bar{z} \qquad (n, i = 0, 1, 2, \ldots)$$

(ii) Use the following algorithm to evaluate $\bar{z}(\bar{t}_{n+1})$ given $\bar{z}(\bar{t}_n)$:

$$\bar{z}(\bar{t}_{n+1}) = z(\bar{t}_n) + \int_{\bar{t}_n}^{\bar{t}_{n+1}} d\bar{t}\, v_C(\bar{z}, \bar{t}) + \sqrt{2}\int_{\bar{t}_n}^{\bar{t}_{n+1}} d\bar{W}(\bar{t})$$

$$\simeq \bar{z}(\bar{t}_n) + \bar{v}_C(\bar{z}(\bar{t}_n), \bar{t}_n) + \sqrt{2}z_{in} \tag{49}$$

where

$$z_{in} = \int_{\bar{t}_n}^{\bar{t}_{n+1}} d\bar{w}(\bar{t}) \tag{50}$$

z_{in} is a Gaussian random variable with $\langle z_{in} \rangle = 0$ and variance

$$\langle z_{in}^2 \rangle = \left\langle \int_{\bar{t}_n}^{\bar{t}_{n+1}} d\bar{W}(\bar{t}) \int_{\bar{t}_n}^{\bar{t}_{n+1}} d\bar{W}(\bar{t}') \right\rangle$$

$$= \int_{\bar{t}_n}^{\bar{t}_{n+1}} d\bar{t} = \Delta t \tag{51}$$

The first step is a purely diffusive motion starting at $t = 0$ and $\bar{v}_C = 0$.

(iii) Repeating the procedure for many trajectories of bacteria one then gets a histogram of $\bar{b}(\bar{z}, \bar{t}_n)$ using intervals of width $\Delta\bar{z}$.

(iv) Knowing $\bar{b}(\bar{z}, \bar{t}_n)$ one gets $\bar{C}(\bar{z}, \bar{t}_{n+1})$ by using a simple approximation

$$\bar{C}(\bar{z}, \bar{t}_{n+1}) \simeq \bar{C}(\bar{z}, \bar{t}_n) - \bar{b}(\bar{z}, \bar{t}_n)\Delta t \tag{52}$$

(v) Compute the derivative $\partial \bar{C}/\partial \bar{z}$ by

$$\frac{\partial \bar{e}}{\partial \bar{z}}(\bar{z}, \bar{t}_{n+1}) \simeq \frac{\partial \bar{C}}{\partial \bar{z}}(\bar{z}, \bar{t}_n) - \left[\bar{b}(\bar{z} + \Delta\bar{z}, \bar{t}_n) - \bar{b}(\bar{z}, \bar{t}_n)\right] \frac{\Delta \bar{t}}{\Delta \bar{z}} \tag{53}$$

(vi) It is then possible to evaluate $\bar{v}_C$ at $\bar{t} = \bar{t}_{n+1}$ for every value of $\bar{z}$ with a 4-point Lagrange interpolation according to the values of $\bar{x}(\bar{t}_n)$.

(vii) The procedure is then iterated to give at each instant not only $\bar{b}(\bar{z}, \bar{t} \mid \bar{z}_0)$ and $\bar{C}(\bar{z}, \bar{t})$ but also $\langle \bar{z}(\bar{t}) \rangle$ and $\langle \bar{z}^2(\bar{t}) \rangle - \langle \bar{z}(t) \rangle^2$ as sums over the trajectories. These are two quantities one relates to the speed and width of the traveling band.

4. RESULTS OF THE SIMULATION

Before we begin discussion of the result it is useful to give an order of magnitude of scales. From our previous experiment[7] we have $v \simeq 1 \times 10^{-4}$ cm/sec and $\mu \simeq 1 \times 10^{-6}$ cm^2/sec. Thus the unit of distance is $z_0 = \mu/v = 0.01$ cm and the unit of time is $t_0 = \mu/v^2 = 100$ sec. These figures are consistent with our observations that the width of a bacterial band is generally about 0.1 cm and it migrates about 100 min and gradually dissipates itself.

Figure 4 depicts two typical trajectories $\bar{z}$ vs. $\bar{t}$. The solid line represents an asymptotic average trajectory $\langle \bar{z} \rangle$ vs. $\bar{t}$. In our scaled unit it has a

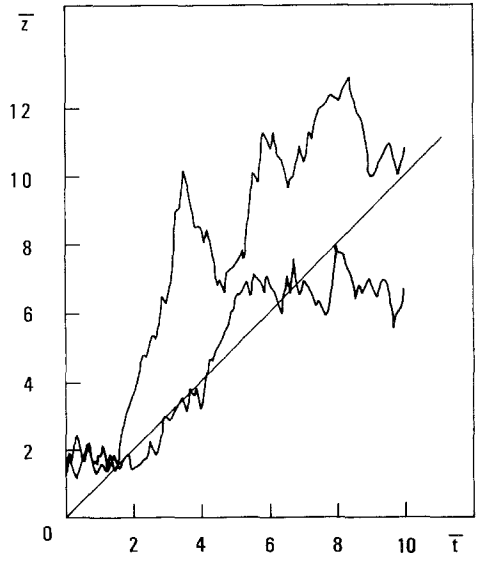

Fig. 4. Typical trajectories of $\bar{z}$ vs. $\bar{t}$.

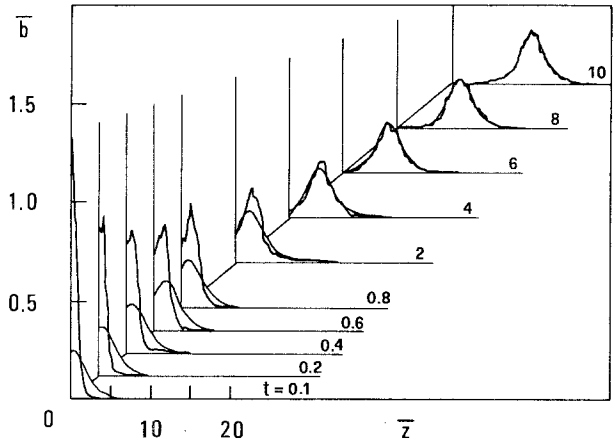

Fig. 5. The band evolution from transient to the steady state.

slope of unity. The time and space intervals $\Delta\bar{t}$ and $\Delta\bar{z}$ used in the simulation are, respectively, 0.01 and 0.1. Figure 5 shows a sequence of development of an initially prepared band $b(z,0) = (N/A)\delta(z)$. As we see the initially sharp band gradually evolves into a K–S steady state band as time goes on. The smooth line drawn under each peak represents the steady state K–S solution. Thus the steady state is reached at $\bar{t} \geqslant 4$, or about 400 sec, which agrees reasonably well with our experimental observation of several minutes. Figure 6 gives plots of $\langle\bar{z}\rangle$ vs. $\bar{t}$ for different $\bar{\delta}$ values

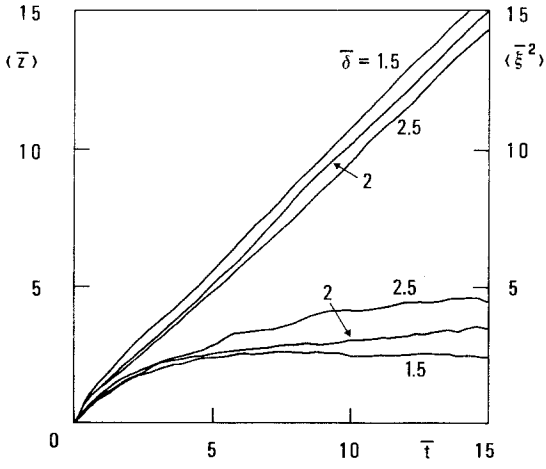

Fig. 6. $\langle\bar{z}\rangle$ vs. $\bar{t}$ and $\langle x^2\rangle$ vs. $\bar{t}$ for different values of $\bar{\delta}$.

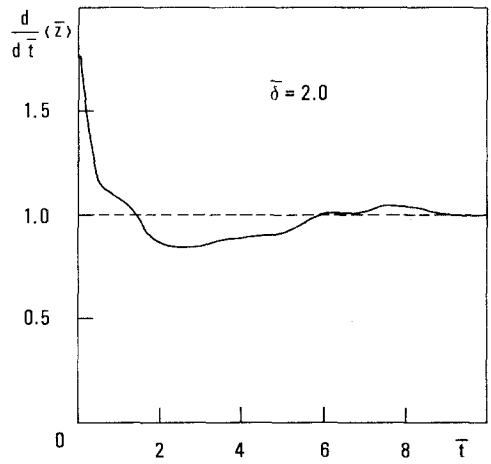

Fig. 7. $d\langle\bar{z}\rangle/d\bar{t}$ vs. $\bar{t}$ for $\bar{\delta} = 2$ case. It shows the approach of v to the steady state value W.

ranging from 1.5 to 2.0. This range corresponds to cases of actual interest.[7] We see that after a transient period of $t \leqslant 4$, the $\langle\bar{z}\rangle$ vs. $\bar{t}$ plots settle down to a constant slope of ~ 1. In the same figure we also give $\langle\bar{\xi}^2\rangle \equiv \langle x^2\rangle$, which is the second moment of the traveling band. This second moment gives a measure of the width of the band which gradually approaches a constant value of the K–S band width as the time increases above $\bar{t} \geqslant 4$. In

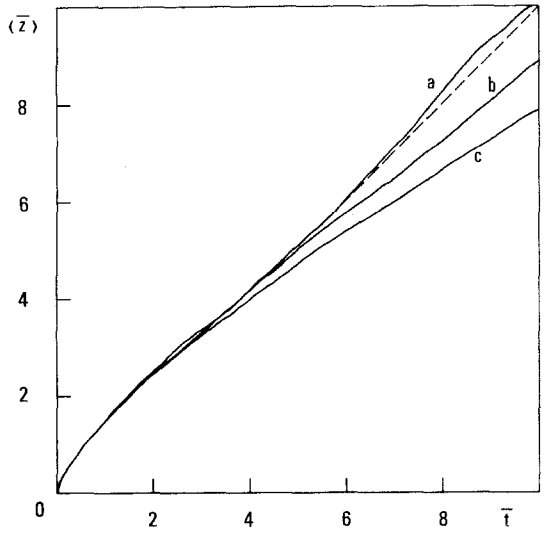

Fig. 8. $\langle\bar{z}\rangle$ vs. $\bar{t}$ for K–S and non-K–S cases.

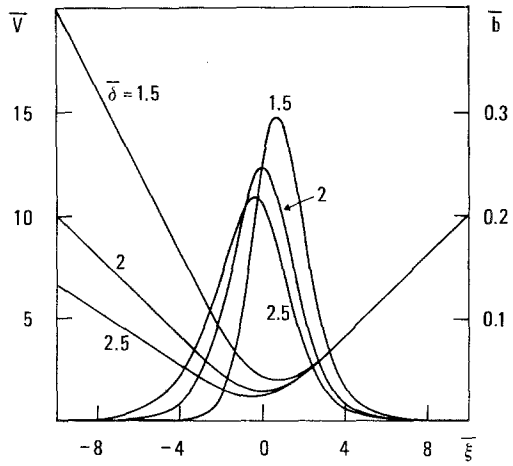

Fig. 9. K–S band locations with respect to the potential V minimum for different values of $\bar{\delta}$.

order to obtain the speed of the band migration we compute $d\langle\bar{z}\rangle/d\bar{t}$ vs. $\bar{t}$. In Fig. 7 we show a case for $\bar{\delta} = 2.0$ in which we can see the speed approach nicely a value unity (equal to W) for $\bar{t} \geqslant 6$.

Figure 8 gives results of simulation for the extended K–S case where $f(\bar{C}) \neq 1$ in comparison with the K–S case where $f(\bar{C}) = 1$. Curve (a) gives the K–S case where $v/W = 1$, (b) gives a case $\bar{C}_T = 0.1$, $\alpha = 0.75$, with a result $v/W = 0.77$, and (c) gives a case $\bar{C}_T = 0.2$, $\alpha = 0.75$ with a result $v/W = 0.63$. As can be seen from Fig. 3, $v/W < 1$ generally for the non-K–S cases.

Figure 9 illustrates the fact that in the steady state K–S case one can interpret the band to sit on a minimum of the potential well V as given by Eq. (44). Putting $\bar{\xi} \equiv x$ it is easy to see that

$$\bar{v}_C = \frac{\bar{\delta}}{\bar{\delta} - 1} \frac{e^{-x}}{1 + e^{-x}} = -\frac{\partial \bar{V}}{\partial \bar{z}} \tag{54}$$

and the minimum of the well is given by x_0, where

$$x_0 = \ln\left(\frac{1}{\bar{\delta} - 1}\right) \tag{55}$$

5. CONCLUSION

We showed that the model equations of Chemotaxis proposed by Keller and Segel[6] can be extended to take into account the concentration

dependence $k(c)$ of the consumption rate. We introduced a simple concentrations dependence of v/W to $\bar{C}_T$ and α.

We used a stochastic computer simulation technique to solve for the transient behavior of the K–S model and extended K–S equation. We showed that the transient solution gradually approaches the steady state behavior after $\bar{t} \geqslant 4$. It is of interest to apply this technique also to a case where diffusion of the substrate is nonzero.

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