MATHEMATICAL BIOSCIENCES
AND ENGINEERING
Volume **6**, Number **1**, January **2009**

doi:10.3934/mbe.2009.6.83

pp. **83–91**

COMPUTATION OF TRAVELING WAVE FRONTS FOR A NONLINEAR DIFFUSION-ADVECTION MODEL

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(Communicated by Stephen Gourley)

Abstract. This paper utilizes a nonlinear reaction-diffusion-advection model for describing the spatiotemporal evolution of bacterial growth. The traveling wave solutions of the corresponding system of partial differential equations are analyzed. Using two methods, we then find such solutions numerically. One of the methods involves the traveling wave equations and solving an initial-value problem, which leads to accurate computations of the wave profiles and speeds. The second method is to construct time-dependent solutions by solving an initial-moving boundary-value problem for the PDE system, showing another approximation for such wave solutions.

1. **Introduction.** It is known from Experiments demonstrate that a number of different types of bacterial colonies exhibit different spatial patterns. The nature of these spatial structures depends on the growth medium and on the type of bacteria, which often secrete some chemoattractant. Expansion and growth of the colony are observed. The colony expands and grows, during which bacterial cells migrate toward regions of fresh nutrients and the colony boundary may take on fascinating shapes. Colony expansion is phenomenologically modeled in terms of reaction-diffusion equations for nutrients and bacteria density. These equations may involve cell multiplication and death, linear or nonlinear diffusion, and chemotactic response to nutrients or to other chemicals secreted by the bacteria [5-11,16]. Such models typically reproduce the motion of a wave front corresponding to the boundary of the expanding bacterial colony.

Here we focus on the study of colony pattern exemplified by the growth of bacteria of the type *Paenibacillus dendritiforms* on a thin layer of agar in a Petri dish. These bacteria cannot move on a dry surface and produce a layer of lubricating fluid in which they swim. In a uniform layer of liquid, bacterial swimming is a random process by the bacteria'motion and diffusion, which cause the lubrication fluid to flow. The availability of nutrients affects the reproduction of bacteria, the production of lubricating fluid, and the withdrawal of bacteria into a pre-pore state. The bacteria consume the nutrients. A continuum approach to the dynamics leads to a model, namely, a reaction-diffusion-convection system for the bacteria density

2000 *Mathematics Subject Classification.* Primary: 35K65, 35B25; Secondary: 34C37.
Key words and phrases. reaction-diffusion-advection equations; bacterial growth; traveling wave fronts; numerical approximations.

$b(x, y, t)$ and the nutrient density $n(x, y, t)$:

$$\frac{\partial b}{\partial t} = \nabla \left(D_b \nabla b - b \nabla n \right) + f(n, b), \tag{1.1}$$

$$\frac{\partial n}{\partial t} = D_n \nabla^2 n - g(n, b), \tag{1.2}$$

with D_n describing the diffusion constant of the nutrient, and

$$D_b = D_0 nb, \tag{1.3}$$

implying a density-dependent diffusion coefficient. The reaction term is given by

$$f(n, b) = g(n, b) = nb, \tag{1.4}$$

which in chemical terms is like a bilinear autocatalytic reaction [2]. Then, by replacing $f(n, b)$ and $g(n, b)$ by (1.4) and, for simplicity, taking $D_n = 0$, $D_0 = 1$, we obtain the following one-dimensional reaction-diffusion-convection system

$$\frac{\partial b}{\partial t} = \frac{\partial}{\partial x} \left(nb \frac{\partial b}{\partial x} - b \frac{\partial n}{\partial x} \right) + nb, \tag{1.5}$$

$$\frac{\partial n}{\partial t} = -nb, \tag{1.6}$$

which extends the one system in [14] when chemotaxis term arises in the equation for the bacteria density (1.5).

The main aim of this paper is to study the traveling wave fronts for (1.5)-(1.6) numerically, determining the wave speed and the wave profile, as precisely as possible. These are key issues from biological viewpoint.

The rest of the paper is organized as follows. Section 2 contains analytical results of traveling waves as well as numerical computations. In Section 3 the numerical time-dependent solutions of partial differential equation system are constructed. Finally, Section 4 is devoted to conclusions.

2. **Traveling waves.** If we seek a permanent form traveling wave solution, $b(x, t) = b(y)$, $n(x, t) = n(y)$, $y = x - ct$, c is the constant wave speed, we must solve

$$\frac{d}{dy} \left(nb \frac{db}{dy} - b \frac{dn}{dy} \right) + c \frac{db}{dy} + nb = 0, \tag{2.1}$$

$$c \frac{dn}{dy} = nb, \tag{2.2}$$

subject to the following boundary conditions: far behind the wave

$$b \to 1, \ n \to 0, \ as \ y \to -\infty \tag{2.3}$$

and far ahead of the wave

$$b \to 0, \ n \to 1, \ as \ y \to \infty \tag{2.4}$$

so that the wave is propagating into the nutrient region of the plate.

In order to find traveling wave solutions we use the standard method; namely, we look for heteroclinic trajectories of the associated ordinary differential equation system of (2.1)-(2.2). Adding equations (2.1)-(2.2) and integrating once gives

$$nb \frac{db}{dy} - b \frac{dn}{dy} + c \left(b + n \right) = \text{constant}.$$

The boundary conditions at $\pm\infty$ dictate that the constant of integration is equal to c. Hence, we obtain the first order ODE system

$$nb\frac{db}{dy} = c\,(1-n-b) + \frac{b^2 n}{c}, \tag{2.5}$$

$$\frac{dn}{dy} = \frac{nb}{c}. \tag{2.6}$$

Introducing the variable z such that $d_y z = 1/bn\,(y) > 0$ for all y as in [14], the ODE system (2.5)-(2.6), in terms of z, becomes

$$\frac{db}{dz} = c\,(1-n-b) + \frac{b^2 n}{c}, \tag{2.7}$$

$$\frac{dn}{dz} = \frac{(nb)^2}{c}. \tag{2.8}$$

Given that $1/\,(bn) > 0$ for $b, n > 0$, the dynamics given by (2.5)-(2.6) and those associated with (2.7)-(2.8) are the same. That is, namely, if every solution (b, n) to (2.5)-(2.6) is nonzero everywhere, then (2.5)-(2.6) would be equivalent to (2.7)-(2.8). If this is not the case, then there would a $y_* \in R$ such that

$$by(y_*) = 0.$$

This which implies that $(b+n)(y_*) = 1$. Hence, by assuming that b is monotone decreasing and n is monotone increasing , we obtain $b(y_*) = 0, n(y_*) = 1$ and $b(y) = 0, n(y) = 1$ for all $\infty > y \geq y_*$. Also from (2.1), for this case we obtain $db/dy(y_*) = -c$. The conclusion is that the variables (b, n) approach their limits values as $y \to \infty$ and might reach these values in finite y value. This also will be shown in next subsection.

2.1. **Phase plane analysis.** Note that the behavior of the system (2.7)-(2.8) is entirely equivalent to that of the system (2.5)-(2.6). Then our problem reduces to finding heteroclinic trajectories in the $b-n$ plane between the two steady states $R = (b, n) = (1, 0)$ and $S = (b, n) = (0, 1)$ of (2.7)-(2.8). This is also equivalent to looking for trajectory solutions of the ODE

$$\frac{dn}{db} = \frac{(nb)^2}{c^2\,(1-b-n) + b^2 n}, \tag{2.9}$$

in the form $n = n\,(b) > 0$. Hence, any traveling wave solution of (1.5)-(1.6) corresponds to a solution trajectory of (2.7)-(2.8) or (2.9) connecting the two stationary states $R = (1, 0)$ and $S = (0, 1)$.

At this point, we need to investigate the local behavior of such trajectories near these stationary points by using (2.7)-(2.8) as well as (2.9). A linearization of (2.7)-(2.8) about the stationary state R shows that R is a nonhyperbolic point. The eigenvalues of the Jacobian matrix associated with the system (2.7)-(2.8) at R are $\lambda_1 = 0, \lambda_2 = -c$. The corresponding eigenvectors are $v_1 = \left(1, c^2/(1-c^2)\right)$ with $c > 1$ and $v_2 = (1, 0)$. It is clear that v_2 points toward R so that the trajectory leaving this steady state leave along the v_1 direction and hence any traveling wave solution must originate from R along the v_1 direction. From the center manifold theorem [9,10] and Taylor expansion of (2.9) around $b = 1$, one can obtain an approximation of this trajectory locally around R, in the form

$$n_1^T\,(b) = -n_1\,(1-b) + n_2\,(1-b)^2 + \cdots, \tag{2.10}$$

where $n_1 = c^2/(1-c^2)$, and $n_2 = -n_1/(1-c^2)$.

Similarly, a linearization of (2.7)-(2.8) about the stationary state S shows that S is a nonhyperbolic point and the eigenvalues of the Jacobian matrix associated with (2.7)-(2.8) at S are $\lambda_3 = 0, \lambda_4 = -c$, with the corresponding eigenvectors $v_3 = (1, -1)$ and $v_4 = (1, 0)$. Hence, any traveling wave solutions must end at $S = (0, 1)$. Both v_3 and v_4 point towards S. The center manifold theorem and Taylor expansion of (2.9) around $b = 0$, give the approximation of the trajectory locally around S, in the form

$$n_0^T(b) = 1 - \frac{1}{2c^2}b^2 + \cdots \tag{2.11}$$

or

$$n_0^T(b) = 1 - b + \frac{2}{c^2}b^2 + \cdots \tag{2.12}$$

Hence, in the case of (2.11) we get

$$\frac{db}{dz} \approx -cb + \frac{3b^2}{2c} - \frac{b^4}{2c^3},$$

so that $b \to 0$ as $z \to \infty$, and then (2.5) gives, for $(b, n) \approx (0, 1)$,

$$\frac{db}{dy} \approx -c + \frac{3b}{2c} - \frac{b^2}{2c} + \frac{b^3}{4c^3},$$

so that b gets to zero at a finite value of y, i.e. y_* as mentioned above. For the case of (2.12) we get, instead,

$$\frac{db}{dz} \approx -\frac{b^2}{c} - \frac{b^3}{c} + \frac{2b^4}{c^3},$$

and

$$\frac{db}{dy} \approx -\frac{b}{c} - \frac{2b^2}{c} + \frac{4b^3}{c^3},$$

so that $b \to 0$ as $z \to \infty$ and $y \to \infty$.

Now, both v_3 and v_4 point toward S, so that we have two possible ways to enter S. If the traveling wave solution enters along v_4, then the local form of the trajectory is given by (2.11). In this case, for completeness, in similar way that in [14], one can prove the unique existence of such trajectory between R and S which gives the sharp type solution. If the traveling wave solution enters along v_3, then the decay is along the center manifold whose equation is given locally by (2.12). This is the case of nonsharp waves, and no other type of waves exists.

2.2. **Numerical computations.** In order to determine speeds c, which induce such trajectories, corresponding to traveling wave solutions, we solve the phase trajectory equation (2.9) numerically using an adaptive step Runge-Kutta scheme of order 4 [13] for initial conditions that have been estimated from (2.10). As result, we have computed a unique trajectory from R to S for minimum speed which corresponds to a sharp traveling wave solution, and trajectories corresponding to non-sharp traveling wave solutions as the speed increases beyond the minimum speed. The minimum speed can be computed by using the following iteration scheme

$$c = c - \delta\left(n(b, c) - n_0^T(b, c)\right),$$

where δ is the relaxation factor. The stopping criterion is as follows: choose δ and iterate until $|c - c_{min}| < \epsilon$, where ϵ is some tolerance value. With this, the minimum speed was found to be $c_{min} \approx 1.16$. In Figure 1, we show solution trajectories (a) for different speeds (b) for minimum speed $c_{\min}$ with local forms given by (2.10)-(2.11) (c) for speed $c = 2 > c_{\min}$, with local forms given by (2.10)-(2.12).

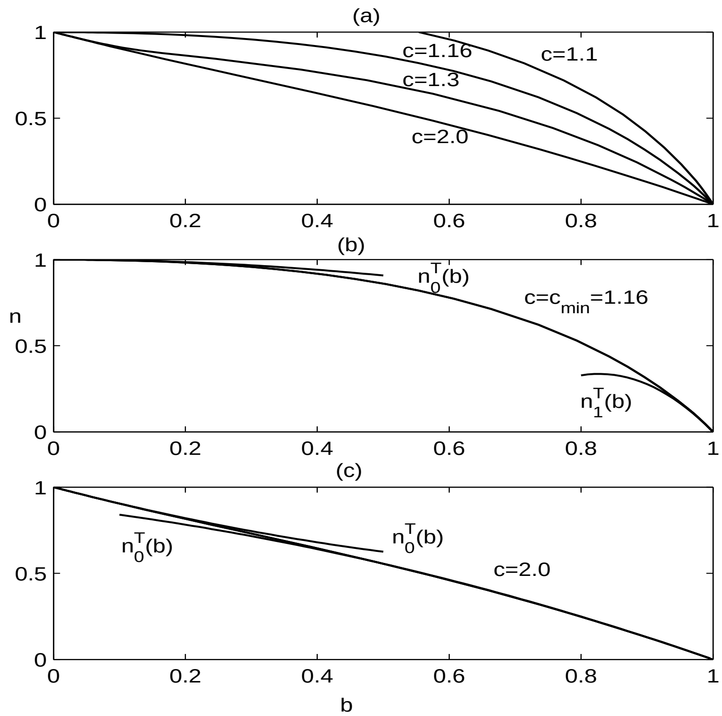

Figure 1. Sketch depicting phase plane trajectories. (a) For different speeds. Clearly for speeds below the minimum speed, there are no trajectories connecting the two steady states. (b) For minimum speed $c_{\min}$ with local forms given by equations (2.10)-(2.11) and (c) for speed $c > c_{\min}$, with the local form (2.10) and the center manifold given by equation (2.12).

In Figure 2, we show a plot of the numerical solutions of (2.5)-(2.6) with minimum speed. We have solved (2.5)-(2.6) for increasing y, using a fourth-order Runge-Kutte method with step size control and initial values of b, n at some finite y, say $y = 0$, have been estimated from (2.10). This figure clearly shows that the b wave front is of sharp type. In Figure 3, we give a plot of numerical solution of (2.5)-(2.6) for speed $c = 2.0 > c_{\min}$, which shows non-sharp wave.

3. **Numerical time-dependent solutions.** In this section we construct the time-dependent solutions of the partial differential equation system problem and show an another numerical approximation for traveling wave solutions of the model equations, in particular, the sharp type wave solution propagating with minimum speed. To do this, we solve (1.5)-(1.6) numerically. These equations (1.5)-(1.6) are all symmetric in x, that is, any spatial localized input of bacteria results in the formation of symmetrically propagating structures, of non-zero bacterial density, to the left and right directions simultaneously, so a symmetry centered at $x = 0$. Therefore, we solve the problem on the semi-infinite spatial domain $K = (x : 0 \leq x \leq \infty)$. We introduce a moving boundary problem, that is, a fixed symmetry boundary condition

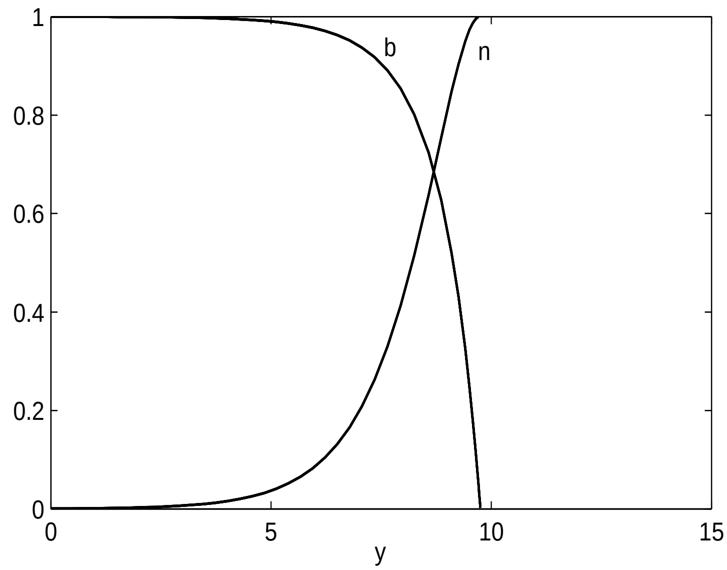

FIGURE 2. Plot of the numerical solutions of (2.5)-(2.6) with minimum speed. This figure shows that a sharp traveling wave front exists whose speed is uniquely determined. Clearly the b profile is of sharp type.

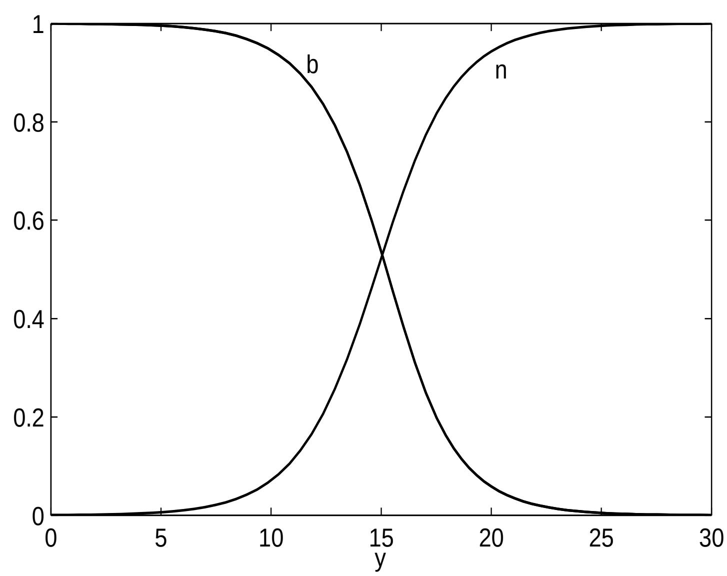

FIGURE 3. Plot of the numerical solutions of (2.5)-(2.6) for speed $c = 2.0$, showing faster, smooth traveling wave solutions.

at $x = 0$ and a moving boundary condition at $x = x_* (t)$, for the PDE system

$$\frac{\partial b}{\partial t} = \frac{\partial}{\partial x}\left(nb\frac{\partial b}{\partial x} - b\frac{\partial n}{\partial x}\right) + nb, \tag{3.1}$$

$$\frac{\partial n}{\partial t} = -nb, \tag{3.2}$$

for $0 < x < x_* (t)$, $t > 0$ with the Dirichlet condition $b = 1$ at $x = 0$. The conditions for the moving boundary $x = x_* (t)$, are $b (t, x_* (t)) = 0$ and,

$$-\frac{dx_*}{dt} = \left(\frac{\partial b}{\partial x} - \frac{\partial n}{\partial x}\right)\Bigg|_{(t,x_*(t))}. \tag{3.3}$$

Equations (3.1)-(3.2) with (3.3) can be solved numerically, as in [4], by mapping the equations with a suitable choice of new space coordinates onto a fixed spatial domain and using finite differences to construct approximate solutions of the transformed equations. For this problem we introduce the transformation

$$\zeta = x - x_* (t) \leq 0. \tag{3.4}$$

Then using (3.4), (3.1)-(3.2) become

$$\frac{\partial b}{\partial t} = \frac{\partial b}{\partial \zeta}\frac{dx_*}{dt} + \frac{\partial}{\partial \zeta}\left(nb\frac{\partial b}{\partial \zeta} - b\frac{\partial n}{\partial \zeta}\right) + nb, \tag{3.5}$$

$$\frac{\partial n}{\partial t} = \frac{\partial n}{\partial \zeta}\frac{dx_*}{dt} - nb, \tag{3.6}$$

for $\zeta \leq 0, t > 0$. In order to solve (3.5)-(3.6) we discretize only the space derivatives and integrate the resulting ordinary differential equations in time along constant $\zeta = \zeta_i$ line. Numerical solutions when the initial conditions are $b (x, 0) = 0, n (x, 0) = 1$ for all $x > 0$, are shown in Figure 4. In this figure we plotted b and n as functions of space x at equal intervals of time, showing the time evolution of sharp traveling wave. The computed value of the wave speed is found to be 1.1386, which is close to the value of the minimum speed predicted in the previous section. We have calculated this speed by computing the velocity of the front position defined by the position of a selected level point on the wave front and the velocity of moving boundary position, where we have found that both equal this approximate value. Moreover, numerical simulations (results not shown) carried out on the PDE system (1.5)-(1.6) for initial conditions have decay of the form $b (x, 0) = \exp (-\alpha x)$, show nonsharp waves with speeds greater than the minimum speed. Notice that this form of wave speed dependence of initial conditions is familiar from parabolic partial differential equations [12, 15].

4. **Conclusion.** In this paper we have considered a nonlinear diffusion-advection model for describing the spatiotemporal evolution of bacterial colony pattern. We analyzed the traveling wave solution of the corresponding system of partial differential equations. We then presented numerical results on the existence of such traveling wave solutions using different methods. We have numerically solved the traveling wave ODE system and computed a minimum wave speed giving a sharp wave. Further, we have numerically constructed the time-dependent solutions of the PDE system showing an approximation of such waves, in particular, sharp wave with minimum speed. In comparison, the obtained solutions from the PDE system are in good agreement with that obtained from phase plane method not only in the wave speed, but also in the wave profile.

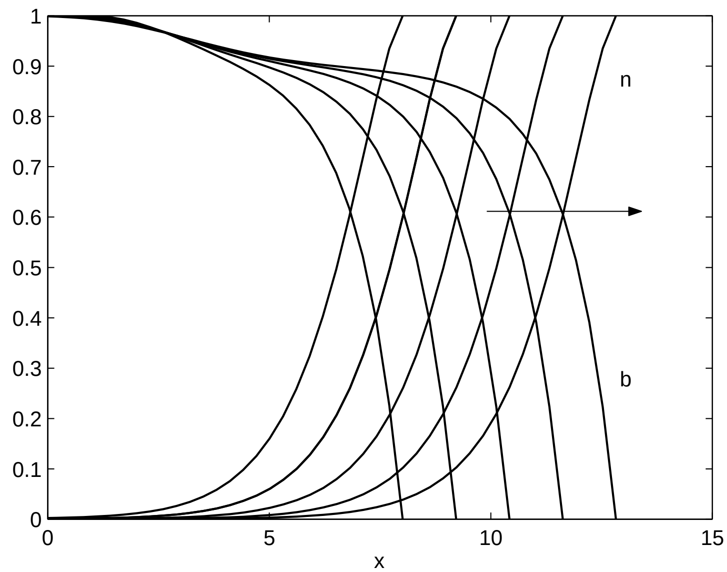

FIGURE 4. Numerical results showing the sharp type solution. In this figure b and n are plotted as functions of space x at equal intervals of time. The arrow shows the direction of increasing time This solution corresponds to a wave front of sharp type with minimum speed.

Acknowledgements. The author thanks the anonymous referee for helpful comments.

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Received November 26, 2007; Accepted August 27, 2008.

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