Modelling Microbial Chemo-tactic Waves Using Adaptive Mesh Refinement

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1 Introduction

Ground-water contaminants often persist in low-permeability regions, in which the flow rate is small. Fortunately, many soil microbes are able to degrade common pollutants and are chemo-tactic, meaning that they can migrate toward chemical concentrations that they find desirable, [1, 2]. In fact they can be highly motile: typical microbe swimming speeds are of order $10^{-3}-10^{-2}$ cm s^{-1}, whereas groundwater flow speeds are in the range $10^{-1} - 10^{-4}$ cm s^{-1}. Chemo-taxis may increase degradation of ground-water contaminants both by drawing microbes into contaminated regions with low ground-water flow rates, and by enabling them to follow contaminant gradients caused by their own consumption of pollutants [3, 4].

In this work, we consider the movement and growth of microbes in a saturated porous medium with zero flow. Specifically, we consider a system of equations that describe the fate and transport of microbes induced by a contaminant gradient (chemo-taxis) and diffusion, and in which their growth and the degradation of the contaminant is described by a Monod kinetics model.

2 Governing equations

The system is described by the following equations

$$\frac{\partial c}{\partial t} = D_c \nabla^2 c - \frac{f(b,c)}{Y} \quad a), \qquad \frac{\partial b}{\partial t} = -\nabla \cdot (b\mathbf{v}) + D_b \nabla^2 b + f(b,c) - d_b b \quad b). \tag{1}$$

Here c is the contaminant concentration, b is the microbe concentration, D_c is the contaminant diffusion coefficient, D_b is the microbe diffusion coefficient, Y is the yield coefficient.

The microbe growth rate is given by Monod kinetics:

$$f(b,c) = \frac{\mu c b}{K_c + c}, \tag{2}$$

where μ is the growth coefficient and K_c is the saturation coefficient. d_b is the microbe death rate.

The chemo-tactic velocity is given by

$$\mathbf{v} = \frac{\chi K_v}{(K_v + c)^2} \nabla c, \tag{3}$$

where χ is the chemo-tactic sensitivity and K_v is the chemo-tactic saturation constant. Note that $\mathbf{v}$ is of the same form as $\nabla(f/b)$.

It is convenient to non-dimensionalise these equations by setting

$$x' = \frac{x}{L},\ y' = \frac{y}{L},\ t' = \frac{t\chi}{L^2},\ c' = \frac{c}{c_0},\ b' = \frac{b}{b_0}. \tag{4}$$

Here L is size of region and c_0, b_0 are the initial concentrations.

The equations then become

$$\frac{\partial c'}{\partial t'} = \frac{1}{P_c} \nabla'^2 c' - \frac{D_g}{Y'} f' \quad a), \qquad \frac{\partial b'}{\partial t'} = -\nabla'(b'\mathbf{v}') + \frac{1}{P_b} \nabla'^2 b' + D_g f' - D_d b' \quad b). \tag{5}$$

where

$$f' = \frac{c'b'}{(K_c/c_0 + c')},\ Y' = \frac{c_0 Y}{b_0},\ \mathbf{v}' = \frac{L}{\chi}\mathbf{v} = \frac{(K_v/c_0)}{(K_v/c_0 + c')^2} \nabla' c', \tag{6}$$

The dimensionless parameters are

Contaminant Peclet No $P_c = \dfrac{\chi}{D_c}$, Microbe Peclet No $P_b = \dfrac{\chi}{D_b}$,

Growth Damköhler No $D_g = \dfrac{\mu L^2}{\chi}$, Death Damköhler No $D_g = \dfrac{d_b L^2}{\chi}$.

For $L = 100$ cm with Pseudomomas Putida consuming naphthalene in a porous medium with beads of size $250 - 300$ μm we get

$P_c = 0.89$, $P_b = 8.9 \times 10^3$, $D_g = 1.3 \times 10^6$, $D_d = 2.1 \times 10^4$.

This tells us that microbe diffusion is negligible compared to contaminant diffusion and microbe death is much less important than microbe growth.

3 Shocks

In one dimension, equations (5) reduce to

$$\frac{\partial c}{\partial t} = -\frac{D_g}{Y} f \quad a), \qquad \frac{\partial b}{\partial t} = -\frac{\partial (v_x b)}{\partial x} + D_g f \quad b). \tag{7}$$

if we neglect diffusion (note that we have suppressed the primes).

Differentiate (7a) to get

$$\frac{\partial}{\partial x}\frac{\partial c}{\partial t} = \frac{\partial c_x}{\partial t} = -\frac{D_g}{Y}\frac{\partial f}{\partial x} \quad \left(c_x \equiv \frac{\partial c}{\partial x} \right). \tag{8}$$

(7b) (without the source term) and (8) constitute a non-linear hyperbolic system whose wave speeds are

$$\lambda_\pm = \frac{1}{2}[v_x \pm \surd(v_x^2 + 4v_x f/c_x)] \tag{9}$$

The shock relations are

$$s(b_l - b_r) = v_{xl}b_l - v_{xr}b_r, \;\; a), \quad s(c_{xl} - c_{xr}) = \frac{D_g}{Y}(f_l - f_r) \;\; b). \tag{10}$$

It can be seen that b and c_x can become discontinuous, whereas c must remain continuous.

4 Simple solution for a chemo-tactic wave

Equations (7) admit chemo-tactic waves, which are analogous to detonation waves. On dimensional grounds we must have

Speed of wave $\propto D_g^{1/2}$, Thickness of wave $\propto D_g^{-1/2}$.

Since D_g is large, this means that the wave are thin.

If the initial contaminant concentration, c_0, is small compared to K_c and K_v, then we can define new units in which

$$f = bc, \quad v_x = \nabla c.$$

In this case we can find a simple solution for a steadily travelling one dimensional chemo-tactic wave.

Let $\xi = x - st$, where s is the speed of the wave. The solution consists of a shock travelling with speed s with $b = 0$ for $\xi > 0$, $b = Y$ for $\xi < 0$. c is given by

$$c = 1 \quad \text{for } \xi > 0, \quad c = \exp\left(\frac{D_g}{s}\xi\right) \quad \text{for } \xi < 0.$$

The speed of the wave is $s = D_g^{1/2}$ and its thickness is $1/D_g^{1/2}$, as expected. Note that the positive wavespeed vanishes in the frame of the wave at $x = -0.6931$ i.e. there is a sonic point. However, unlike a detonation, the reaction rate does not vanish at the sonic point.

5 Numerical scheme

Despite the apparent simplicity of the system, the Riemann problem is quite complicated. However, since there are only two waves, it is eminently suited to an HLL scheme. The diffusive fluxes can be calculated with a with central difference, as usual. However, there remains the problem of calculating ∇c for the chemo-tactic term. There are two obvious possibilities:

Method 1: Get ∇c by numerical difference of c. This works well enough if the waves are well resolved, but it is not properly upwind. However, it is simple and introduces no extra variables.

Method 2: Take the gradient of the c equation, define new variables ∇c and solve the resulting equation. Although this gives better shock capturing, it has more variables and the numerical solutions for c and ∇c are not automatically compatible.

We therefore opt for method 1.

Figure 1 shows a comparison between the numerical and exact solutions for $D_g = 1.0$. It is clear that the agreement is very good except for a slight lack of monotonicity at the shock, which is a consequence of opting for method 1. The numerical wave speed is 0.994, which is is very close to the exact wave speed of 1.

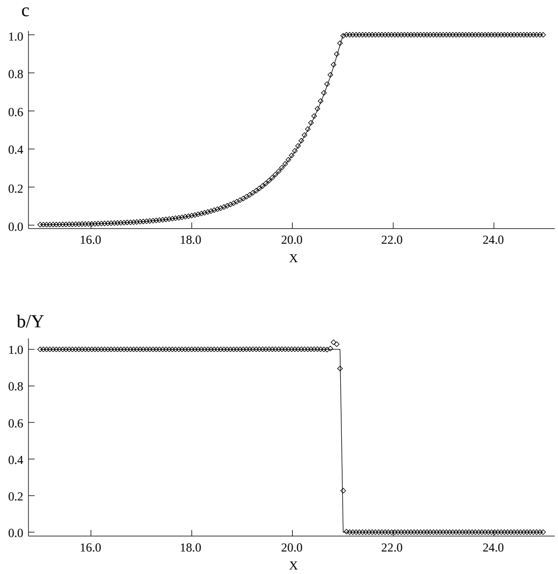

Figure 1: Simple one dimensional chemo-tactic wave. The line is the exact solution, the markers from the numerical calculation

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6 Realistic one dimensional chemo-tactic wave

Figure 2 shows the numerical solution for a wave with the parameters discussed in section 2, except that microbial death is neglected since it has no effect on the wave. Note that $Y = 0.538$. The lower resolution run (markers) had $\Delta x = 12.8 \times 10^{-6}$ and gave a wave speed of 2.0728×10^3, whereas the higher resolution run (line) had $\Delta x = 6.4 \times 10^{-6}$ and a wave speed of 2.0732×10^3. These were computed using a cell-by-cell adaptive mesh refinement (AMR) code [5] with 4 grid levels for the lower resolution calculation and 5 levels for the higher one. As one would expect, the large Peclet number for microbial diffusion means that the shock structure is very thin and is only just resolved in the higher resolution calculation. The entire wave is also very thin because of the large Damköhler number for microbial growth. If one translates this back into physical units, then the wave thickness is $\simeq 0.05$ cm and its speed is 2.76×10^{-5} cm s^{-1}.

7 Realistic wave in a petri dish

Having established that the numerical method works well in one dimension, we now consider a circular wave, such as the ones that are observed in laboratory experiments in Petri dishes. The initial conditions were $c = 1$, $b = Y$ in $0 \leq r \leq 0.001$, 0 elsewhere. The size of the domain is appropriate for a 3 inch Petri dish. This was an AMR calculation with 6 grid levels giving with a minimum mesh spacing of 12.8×10^{-6}. At the final time the filling factor of the finest grid was 0.0023, which means that the calculation is extremely efficient. It would clearly be extremely expensive to carry out such a calculation with a uniform grid.

Figure 3 shows the wave speed as a function of time. It is clear that the wave takes a while to accelerate and even at later times, there is a curvature effect. Nevertheless, the final speed is quite close to the one dimensional value.

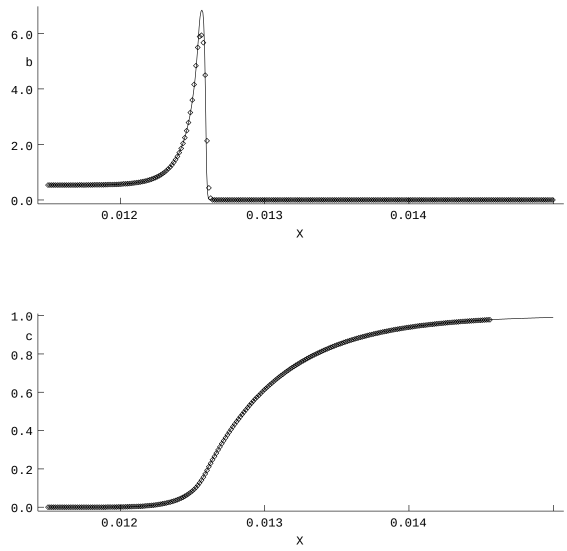

Figure 2: High (line) and low (markers) numerical solution for a realistic one dimensional chemo-tactic wave.

8 Groundwater pollution

It can be seen that it is quite difficult to model a wave even on the scale of a Petri dish. In groundwater problems, the polluted region may have a scale of many kilometres, which means that it is quite impossible to model the real wave, even with AMR.

Since the wave is one-dimensional, one could use a one dimensional calculation to get the wave speed and then use a level set method. The alternative is to use the simple model with an increased wave thickness, combined with AMR.

To do this, all we have to do is to multiply the chemo-tactic term by a factor, α. We then have

$$\text{wave speed} = (\alpha D_g)^{1/2}, \quad \text{wave thickness} = (\alpha / D_g)^{1/2}.$$

Now choose α, D_g to get desired thickness and correct wave speed. The only restriction is that the thickness of the wave should be sufficiently small compared to the scale of the polluted region for curvature effects to be neglible.

9 Conclusion

We have shown that it is possible to construct an efficient upwind scheme to model chemo-taxis, but that even chemo-tactic waves on the scale of Petri dishes require very high resolution. AMR is an effective way of doing this, but even so, it is not possible to model the real wave in polluted groundwater. However, it is possible to construct a simple model that propagates the wave at the correct speed. In this simple model the wave thickness is artificially increased, but the use of AMR makes it possible to keep its thickness small compared to the overall scale of the polluted region.

In the absence of diffusion, the chemo-tactic wave has much in common with detonation in that there is a shock at the leading edge and a sonic point in the wave structure. There are, however, some differences:

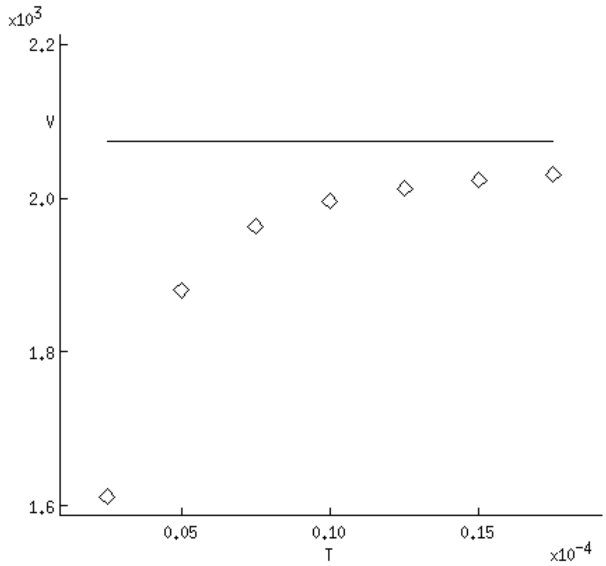

Figure 3: Numerical wave speed for the circular chemo-tactic wave (markers). The line shows the one dimensional speed.

there is no singularity at the sonic point, the reaction rate does not vanish there and the downstream state can affect the wave in the presence of diffusion.

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