A Geometric Construction of Traveling Waves in a Bioremediation Model

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Abstract

Bioremediation is a promising technique for cleaning contaminated groundwater and soil. We study a bioremediation model involving a substrate (contaminant to be removed), electron acceptor (added nutrient), and microorganisms in a 1-D soil column. Using geometric singular perturbation theory, we construct traveling waves (TW) corresponding to motion of a Biologically Active Zone, in which the microorganisms consume both substrate and acceptor. For certain values of the parameters, the traveling waves exist on a 3-dimensional slow manifold within the 5-dimensional phase space. In order to prove persistence of the slow manifold under perturbation, we control the nonlinearity via a change of coordinates and construct the wave in the transverse intersection of appropriate stable and unstable manifolds. We study how the TW depends on the half saturation constants and other parameters.

Introduction

We begin with the nondimensional form of the bioremediation model studied in [1] and [2]. The model assumptions are

- One dimensional, infinite soil column.
- Initial constant level of substrate (S) and biomass (M), and no acceptor (A).
- Constant level of A injected continuously at inlet of soil column.
- S is sorbing: travels at the retarded velocity $1/R_d < 1$.
- Microbes attached to soil particles: no spatial motion.
- M will increase above its equilibrium in the presence of both S and A.

The model equations are

$$\begin{aligned} R_d\frac{\partial S}{\partial t} - \frac{\partial^2 S}{\partial x^2} + \frac{\partial S}{\partial x} &= -a_1 f_{bd} \\ \frac{\partial A}{\partial t} - \frac{\partial^2 A}{\partial x^2} + \frac{\partial A}{\partial x} &= -a_1 a_2 f_{bd} \\ \frac{\partial M}{\partial t} &= a_3 f_{bd} - a_4(M-1) \\ f_{bd} &= M\left(\frac{S}{K_S+S}\right)\left(\frac{A}{K_A+A}\right), \end{aligned}$$

for $x \in [0,\infty)$, $t > 0$, with boundary and initial data

$$\begin{aligned} S(x,0) &= 1; \qquad \left(-\frac{\partial S}{\partial x} + S\right)_{x=0} = 0 \\ A(x,0) &= 0; \qquad \left(-\frac{\partial A}{\partial x} + A\right)_{x=0} = 1 \\ M(x,0) &= 1. \end{aligned}$$

f_{bd} represents monod reaction kinetics. The parameters K_S and K_A represent the relative half-saturation constants and indicate the degree to which the presence of each (or lack thereof) may limit the growth of the microorganisms.

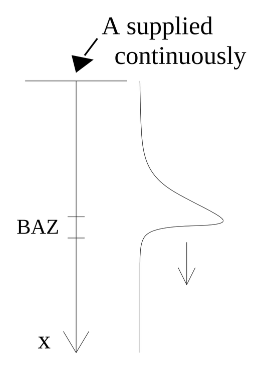

Figure 1a Schematic diagram of the soil column and traveling wave.

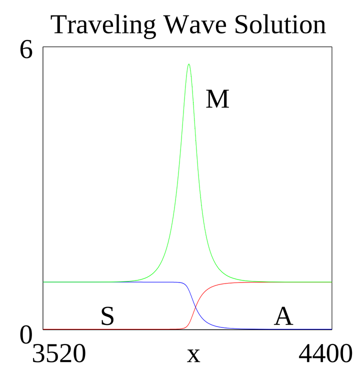

Figure 1b Numerically observed traveling wave solution for $K_S = K_A = 0.3$.

Wave Speed and Scalings

In the TW coordinate $\xi = x - ct$, the model is

$$\begin{aligned} s_{\xi\xi} + (cR_d - 1)s_\xi &= a_1 f_{bd} \\ a_{\xi\xi} + (c-1)a_\xi &= a_1 a_2 f_{bd} \\ cm_\xi &= a_4(m-1) - a_3 f_{bd}, \end{aligned}$$

with asymptotic conditions

$$\begin{aligned} s(-\infty) &= 0, \quad s(+\infty) = 1 \\ a(-\infty) &= 1, \quad a(+\infty) = 0 \\ m(-\infty) &= 1, \quad m(+\infty) = 1. \end{aligned}$$

One may eliminate f_{bd} from the equations for s and a, integrate once with respect to ξ, and use the asymptotic conditions to obtain [1]

$$c = \frac{a_2+1}{a_2 R_d + 1}.$$

We rescale the parameters as suggested by the specific values which produce the numerically observed traveling wave.

$$\begin{aligned} a_1 &= \delta^2 \tilde{a}_1 & R_d &= R_d \\ a_2 &= a_2 & K_S &= \delta^\kappa \tilde{K}_S \\ a_3 &= \delta \tilde{a}_3 & K_A &= \delta^\kappa \tilde{K}_A \\ a_4 &= \delta^2 \tilde{a}_4 \end{aligned}$$

Hence, the model we study is

$$\begin{aligned} s_\xi &= v \\ v_\xi &= -(cR_d - 1)v + \delta^2 \tilde{a}_1 f_{bd} \\ a_\xi &= r \\ r_\xi &= -(c-1)r + \delta^2 \tilde{a}_1 a_2 f_{bd} \\ m_\xi &= \delta^2 \frac{\tilde{a}_4}{c}(m-1) - \delta\frac{\tilde{a}_3}{c} f_{bd}. \end{aligned} \qquad (*)$$

Reduction to Slow Manifold

We cannot apply Fenichel theory directly to the above system because the kinetic terms $\frac{s}{\delta^\kappa \tilde{K}_S + s}$ and $\frac{a}{\delta^\kappa \tilde{K}_A + a}$ in the reaction function f_{bd} are not uniformly bounded in the C^1 topology as $\delta \to 0$. More precisely,

$$\frac{d}{ds}\left(\frac{s}{\delta^\kappa \tilde{K}_S + s}\right) = \frac{\delta^\kappa \tilde{K}_S}{(s + \delta^\kappa \tilde{K}_S)^2} \to \infty \quad \text{for} \quad s \ll \mathcal{O}(\delta^{\frac{\kappa}{2}}).$$

Therefore, we change coordinates to

$$y = \frac{s}{K_S + s}, \qquad w = \frac{a}{K_A + a},$$

which makes the reaction function a polynomial in the new variables.

In addition, we scale the dependent variables as $v = \delta^{1+\kappa}\tilde{v}$, $r = \delta^{1+\kappa}\tilde{r}$, and $m - 1 = \delta^{\kappa-1}\tilde{m}$. System (*) becomes

$$\begin{aligned} y' &= \delta\frac{\tilde{v}}{\tilde{K}_S}(1-y)^2 \\ \tilde{v}' &= -(cR_d - 1)\tilde{v} + \tilde{a}_1\tilde{m}yw + \delta^{1-\kappa}\tilde{a}_1 yw \\ w' &= \delta\frac{\tilde{r}}{\tilde{K}_A}(1-w)^2 \\ \tilde{r}' &= -(c-1)\tilde{r} + \tilde{a}_1 a_2 \tilde{m}yw + \delta^{1-\kappa}\tilde{a}_1 a_2 yw \\ \tilde{m}' &= -\delta\frac{\tilde{a}_3}{c}\tilde{m}yw - \delta^{2-\kappa}\frac{\tilde{a}_3}{c}yw + \delta^2\frac{\tilde{a}_4}{c}\tilde{m}. \end{aligned}$$

The fast variables are $\tilde{v}$ and $\tilde{r}$; the slow variables are y, w, and $\tilde{m}$. There exists a three dimensional slow manifold $\mathcal{M}_\delta$ given by

$$\begin{aligned} \tilde{v} &= h_0(\tilde{m},y,w) + \delta^{1-\kappa}h_1(\tilde{m},y,w) + \delta h_2(\tilde{m},y,w) + \text{h.o.t} \\ \tilde{r} &= g_0(\tilde{m},y,w) + \delta^{1-\kappa}g_1(\tilde{m},y,w) + \delta g_2(\tilde{m},y,w) + \text{h.o.t}, \end{aligned}$$

where $h_0 = -g_0$, $h_1 = -g_1$, and $h_2 = a_2 g_2$. In terms of the slow "time" scale $\eta = \delta\xi$, the motion on $\mathcal{M}_\delta$ is

$$\begin{aligned} y_\eta &= yw\frac{\tilde{a}_1(1-y)^2}{\tilde{K}_S(cR_d - 1)}\left[\tilde{m} + \delta^{1-\kappa} + \delta h_2\right] \\ w_\eta &= -yw\frac{\tilde{a}_1(1-w)^2}{\tilde{K}_A(cR_d - 1)}\left[\tilde{m} + \delta^{1-\kappa} + \delta g_2\right] \\ \tilde{m}_\eta &= -\frac{\tilde{a}_3}{c}yw\left[\tilde{m} + \delta^{1-\kappa}\right] + \delta\frac{\tilde{a}_4}{c}\tilde{m}. \end{aligned} \qquad (**)$$

From the reduced fast dynamics, if a solution leaves the slow manifold it cannot return, and one of $\tilde{v}$ or $\tilde{r}$ must become unbounded as $\xi \to \pm\infty$. Hence, we conclude that the entire TW solution lies on $\mathcal{M}_\delta$.

The expansions for $\tilde{v}$ and $\tilde{r}$ on $\mathcal{M}_\delta$ are not well ordered for $\kappa \geq 1$. Therefore, our construction will be valid only in the regime $0 < \kappa < 1$. This is verified numerically in figure 2.

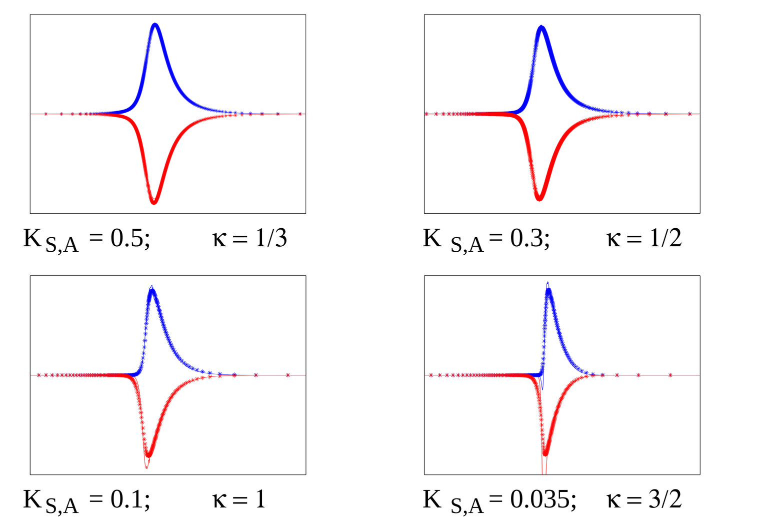

Figure 2. Comparison of v (blue) and r (red) as computed numerically (*) and analytically on the slow manifold (-).

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Determination of Leading Order TW

$N_0^- \equiv \{y = 0\}$ and $N_0^+ \equiv \{w = 0\}$ are "superslow" invariant manifolds of (**). The dynamics on these manifolds are given by

$$y_\zeta = 0, \quad w_\zeta = 0, \quad \tilde{m}_\zeta = \frac{\tilde{a}_4}{c}\tilde{m}, \quad \text{where} \quad \zeta = \delta\eta.$$

These dynamics on N_0^- and N_0^+ correspond to the portions of the TW behind and ahead of the BAZ, respectively.

To capture the dynamics within the BAZ, we use the fact that the $\mathcal{O}(1)$ and $\mathcal{O}(\delta^{1-\kappa})$ terms in (**) imply that

$$\frac{\tilde{K}_S}{(1-y)^2}y_\eta = -\frac{\tilde{K}_A}{(1-w)^2}w_\eta = -\frac{c\tilde{a}_1}{\tilde{a}_3(cR_d - 1)}\tilde{m}_\eta.$$

Using these and the boundary conditions, we compute the integral curves which, combined with the pieces on $N_0^\pm$, determine the leading order traveling wave. The result is shown in figure 3a.

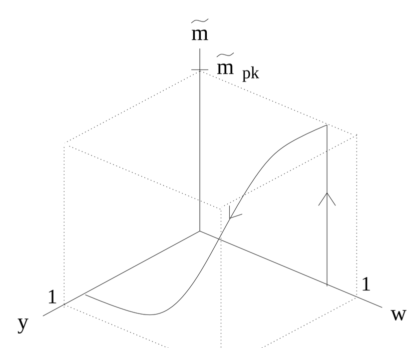

Figure 3a. Sketch of the leading order integral curve near the wave.

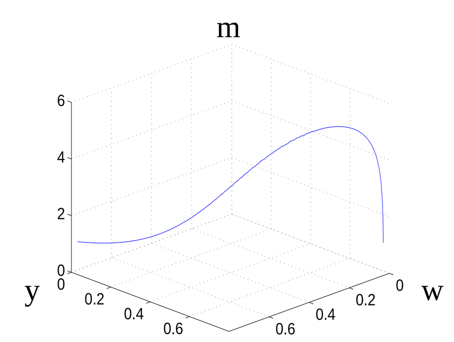

Figure 3b. A plot of the numerically computed traveling wave for $K_{S,A} = 0.3$.

Tracking Manifolds

To prove existence of the wave, we track the following lines and show they intersect transversely the plane $\{y = w\}$ (see figures 4a and 4b):

$$\begin{aligned} L^- &= \{(0, w_-, \tilde{m}) : w_- \text{ fixed}, \quad \tilde{m} \in [0, \tilde{m}_{pk}]\}, \\ L^+ &= \{(y_+, 0, 0) : y_+ \in (1-\epsilon, 1+\epsilon)\}. \end{aligned}$$

Because L^- is the unstable manifold of $(0, w_-, 0)$ in N_0^- and L^+ is a line of equilibria, this result will show that there exists a persistent solution connecting $(0, w_-, 0)$ with one of the points in L^+.

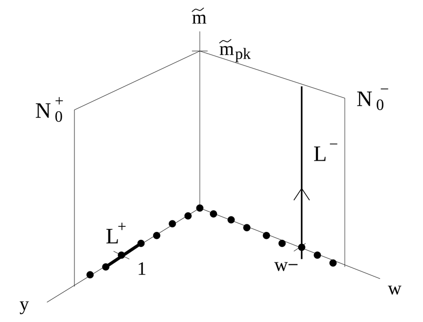

Figure 4a. Schematic diagram of the phase space in $\mathcal{M}_\delta$ and the lines $L^\pm$.

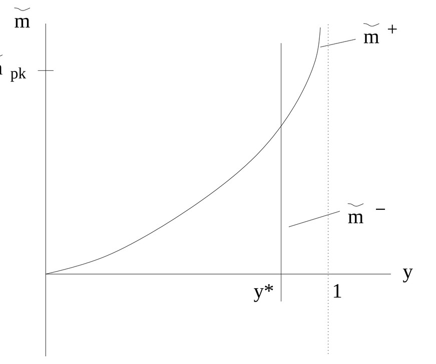

Figure 4b. Sketch of the image of $L^\pm$ in the plane $\{y = w\}$, showing the transverse intersection.

The boundary conditions are satisfied because they are encoded in the wave speed.

Peak Height Dependence on K_S and K_A

It is observed numerically that the peak height of m decreases as κ decreases (as $K_{S,A}$ increase). To leading order, the peak height is constant. However, with the first order corrections, the peak height does decrease with κ. Figure 5a shows agreement between the asymptotics and numerics.

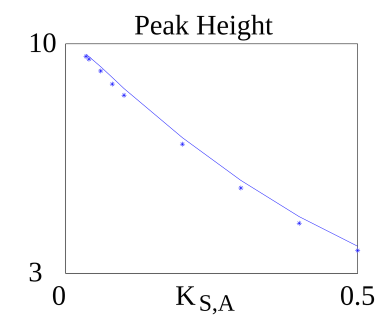

Figure 5a. Comparison of the numerically (*) and analytically computed peak height for m.

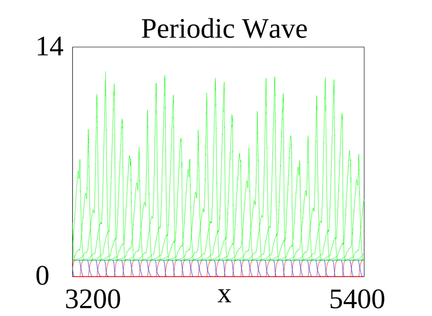

Figure 5b. Numerically computed periodic wave for $K_{S,A} = 0.01$. (See below.)

Conclusions and Work in Progress

We constructed the traveling wave solution within the three-dimensional slow manifold for $K_{S,A}$ sufficiently large. For smaller values, the geometry of the phase space changes, and different analysis must be used in the construction. Future work includes completion of the geometric construction for these parameter values and analyzing the stability of the wave and its bifurcation (see figure 5b).

[1] S. Oya and A. J. Valocchi, Characterization of Traveling Waves and Analytical Estimation of Pollutant Removal in One-dimensional Subsurface Bioremediation Modeling, *Water Resources Research* **33** (1997) 1117–1127

[2] R. Murray and J. X. Xin, Existence of Traveling Waves in a Bioremediation Model for Organic Contaminants, *SIAM J. Math. Anal.* **30** (1998) 72–94

[3] M. Beck, A. Doelman, and T. J. Kaper, A Geometric Construction of Traveling Waves in a Bioremediation Model, (in preparation)