Kinetic model of biofilm formation

immediate

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Part I

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1 Introduction

Consider a static liquid media with air-liquid interface (or glass-liquid). Media is populated by the cells of type S (swimming), ALI is populated by cells of type A (attached). The population of S-type cells is characterized by their density $S(x,t)$ changing with depth (x) and time (t). The depth changes from 0 (ALI) to L (the bottom). The population of A-type cells is characterized by its number at ALI $A(t)$ changing with time. S-type cells can grow with the rate w_S, diffuse with coefficient D, and attach to the ALI at the border with coefficient κ becoming cells of A-type. A-type cells just grow with the rate w_A.

2 Stochastic process to descibe reactive boundary

This simple reactive-diffusion model can be described using deterministic partial-differential equation or stochastic simulation algorithms. These both approaches provide same description of the reactive-diffusion process far from the reactive boundary at the interface, but the behavior close to the reactive boundary is dependent on selected stochastic process (Erban and Chapman 2007).

Here we consider a stochastic simulation algorithm on the lattice size $[0, L]$ (Erban and Chapman 2007). We consider a system with N particles of the planktonic type S on the lattice lattice grids spaced h distance apart. We choose the interval step Δt so it satisfies stability condition $(2D\Delta t \ll h^2)$. The position of i-th molecule at the time t is equal to $x_i(t)$. The position $x_i(t+\Delta t)$ is computed as follows.

$$x_i(t+\Delta t) = \begin{cases} x_i(t), & \text{probability} = 1 - \frac{2D\Delta t}{h^2} \\ x_i(t) + h, & \text{probability} = \frac{2D\Delta t}{h^2} \\ x_i(t) - h, & \text{probability} = \frac{2D\Delta t}{h^2} \end{cases} \tag{1}$$

If molecule hits the boundary $x = 0$, it is adsorbed with probability $P_1 h$ or reflected otherwise. Here P_1 is non negative constant.

Let the probability finding a cell in the bulk satisfies.

$$p_k(t+\Delta t) = (1 - \frac{2D\Delta t}{h^2}) \cdot p_k(t) + \frac{2D\Delta t}{h^2} \cdot (p_{k+1}(t) + p_{k-1}(t)) \tag{2}$$

Passing the limit $\Delta t \to 0, h \to 0$ equation (2) we obtain diffusion equation.

$$\frac{p_k(t+\Delta t) - p_k(t)}{\Delta t} = D\frac{p_k(t) + p_{k-1}(t) - 2p_k(t)}{h^2} \tag{3}$$

$$\frac{\partial n(x,t)}{\partial t} = D \cdot \bigtriangledown^2 n(x,t) \tag{4}$$

Where $n(x,t)$ is a concentration of particles in space x and time t.

The boundary condition can be incorporated into equation as

$$p_1(t+\Delta t) = (1 - \frac{2D\Delta t}{h^2}) \cdot p_1(t) + \frac{D\Delta t}{h^2} \cdot (p_2(t) + (1 - P_1 h)p_1(t)) \tag{5}$$

This equation can be rewritten as

$$\sqrt{\Delta t} \cdot \frac{p_1(t+\Delta t) - p_1(t)}{\Delta t} = \frac{D \cdot \sqrt{\Delta t}}{h} \cdot \left(\frac{p_2(t) - p_1(t)}{h} - P_1 p_1(t) \right) \quad (6)$$

Passing the limit $\Delta t \to 0, h \to 0$ such that $\sqrt{\Delta t}/h$ is kept constant we obtain boundary condition as

$$D \frac{p_2(t) - p_1(t)}{h} = P_1 D \cdot p_1(t) \quad (7)$$

$$D \cdot \frac{\partial n}{\partial x}(x=0,t) = P_1 D \cdot n(x=0,t) \quad (8)$$

Note that P_1 is a given non-negative constant and $P_1 h$ is probability of adsorbtion, where h is a grid size.

3 Kinetic equations

The dynamics of S-type is given by the equation

$$\frac{\partial}{\partial t} S(x,t) = w_S S(x,t) + D \frac{\partial^2}{\partial x^2} S(x,t) \quad (9)$$

with boundary conditions

$$\begin{cases} D \frac{\partial}{\partial x} S(0,t) = P_1 D \cdot S(0,t), & \text{partially adsorbing boader} \\ \\ \frac{\partial}{\partial x} S(L,t) = 0, & \text{reflective boader} \end{cases} \quad (10)$$

where w_S is a grownth rate of the S-type, D is a diffusion coefficient, P_1 is a non-negative constant. At $P_1 = 1$, the boundary condition becomes absorbing $S(0,t) = 0$. At $P_1 = 0$, the boundary condition becomes reflective $\frac{\partial}{\partial x} S(0,t) = 0$.

The growth dynamics of A-type is given by the equation

$$\frac{\partial}{\partial t} A = w_A A + P_1 D \cdot S(0,t). \quad (11)$$

Where w_A is a growth rate of A-type, term $P_1 D \cdot S(0,t)$ is transition flux from S-type to A-type.

4 Analytical solution

We look for solution of the form $S(x,t) = X(x)T(t) \cdot e^{w_S t}$. By substitution $S(x,t)$ into the PDE Eq. (9) and solving for X(x)T(t) we get.

$$\frac{T'}{DT} = \frac{X''}{X} = -\lambda^2 \quad (12)$$

As a result we get

$$S(x,t) = e^{w_S t - \lambda^2 D t} \left(B sin(\lambda x) + C cos(\lambda x) \right) \quad (13)$$

Where A, B and λ are arbitrary.

The next step is to find a certain subset of solutions that satisfy boundary conditions Eq. (10). To do this we substitute (13) to the (10).

$$\begin{cases} D\lambda B = P_1 DC \\ B\lambda cos(\lambda L) - C\lambda sin(\lambda L) = 0 \end{cases} \tag{14}$$

Last equations give us the condition on λ.

$$tan(\lambda L) = \frac{P_1}{\lambda} \tag{15}$$

To find λ we must find the intersection of the curves $tan(\lambda L)$ and P_1/λ.

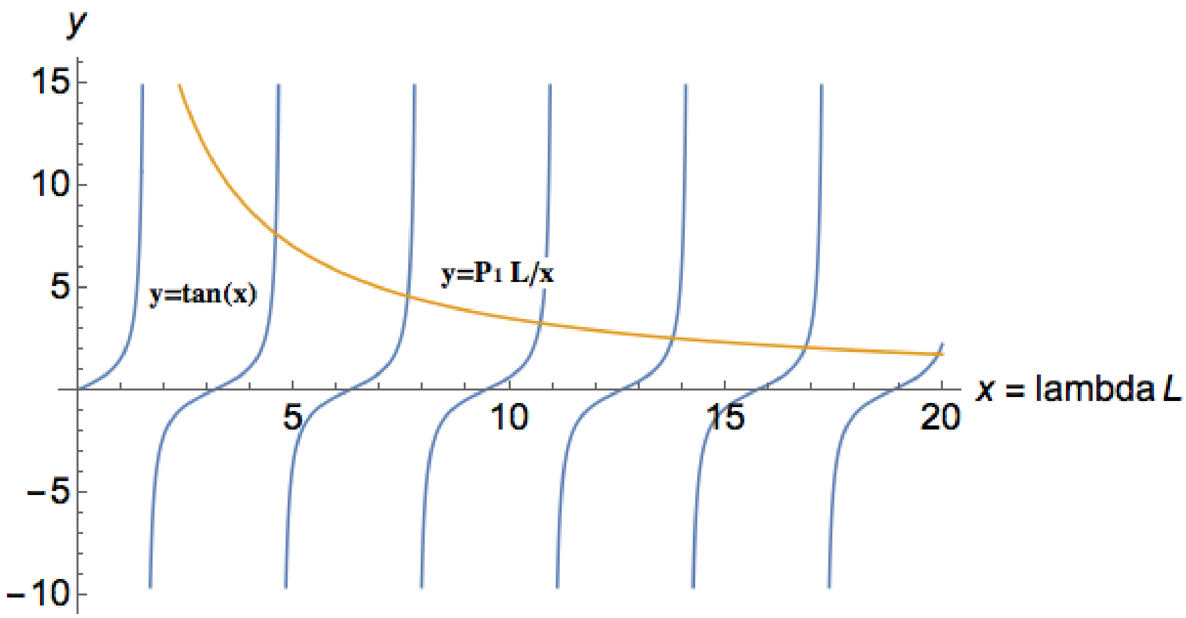

Figure 1: $\lambda_1, \lambda_2, \lambda_3$... are the intersection of the curves $tan(\lambda L)$ and $P_1 L/\lambda L$

These values $\lambda_1, \lambda_2, \lambda_3$... can be computed numerically and called eigenvalues of the boundary-value problem. In other words, they are values of λ for which nonzero solution exsist.
So we have found an infite number of fundamental solutions such as

$$S_n = e^{w_S t - \lambda^2 D t} \left(B_n sin(\lambda_n x) + C_n cos(\lambda_n x) \right) \tag{16}$$

Each of this solution satisfies PDE and boundary condition. The analytical solution for $S(x,t)$ is

$$S(x,t) = \sum_{n=1}^{\infty} e^{w_S t - \lambda_n^2 D t} \left(B_n sin(\lambda_n x) + C_n cos(\lambda_n x) \right) \tag{17}$$

We pick B_n, C_n to satisfy the initial condition.$S(x,0) = f(x)$

$$f(x) = \sum_{n=1}^{\infty} \left(B_n sin(\lambda_n x) + C_n cos(\lambda_n x) \right) \tag{18}$$

$$\frac{\partial}{\partial t} A = w_A A + P_1 D \cdot \sum_{n=1}^{\infty} e^{w_S t - \lambda_n^2 D t} C_n. \tag{19}$$

5 Stationary solution

5.1 S-type

The fundamental solution Eq. (16) has a decay term $e^{-\lambda_n^2 Dt}$ The smallest value of λ_n - λ_1 determine behaviour of the system at the stationary regime. To get λ_1 the Eq. (20) equation should be solved numerically.

$$tan(x) = \frac{P_1 L}{x} \tag{20}$$

$$\tag{21}$$

where $x = \lambda L$

However, some approximation can be done. If $P_1 L >> 1$ then we can use the fact that $tan(\pi/2) = \infty$

$$\lambda = \frac{\pi}{2L} \tag{22}$$

$$S_1 = e^{w_S t - \frac{\pi^2}{4L^2} Dt} (B_1 sin(\lambda x) + C_1 cos(\lambda x)) \tag{23}$$

Note if $D > \frac{4L^2 w_S}{\pi^2}$ S-type fades away.

If $P_1 L << 1$ then we can use the fact that $tan(x) \approx x$

$$\lambda = \sqrt{\frac{P_1}{L}} \tag{24}$$

$$S_1 = e^{w_S t - \frac{P_1}{L} Dt} (B_1 sin(\lambda x) + C_1 cos(\lambda x)) \tag{25}$$

Note if $P_1 > \frac{w_S L}{D}$ S-type fades away.

5.2 A-type

Stationary solution for A-type.

$$\frac{\partial}{\partial t} A = w_A A + P_1 D \cdot \sum_{n=1}^{\infty} e^{w_S t - \lambda_n^2 Dt} C_n. \tag{26}$$

Subsitute $\lambda = \lambda 1$ and $x = 0$

$$\frac{\partial}{\partial t} A = w_A A + P_1 D e^{w_S t - \lambda_1^2 Dt} \cdot C. \tag{27}$$

Where C depends on the initial conditions.

We look for solution in a form $A(t) = f(t) e^{\lambda_S t}$ where $\lambda_S = w_S - \lambda_1^2 D$.

$$f'(t) + (\lambda_S - w_A) f(t) - k = 0. \tag{28}$$

where $k = P_1 DC$

$$f(t) = De^{-(\lambda_S - w_A)t} + \frac{k}{(\lambda_S - w_A)} \tag{29}$$

Taking into account $f(0) = 0$, $D = -\frac{k}{\lambda_S - w_A}$

$$f(t) = \frac{k}{(\lambda_S - w_A)} \left(1 - e^{-(\lambda_S - w_A)t}\right) \tag{30}$$

As a result

$$A(t) = \frac{k}{(\lambda_S - w_A)} \left(1 - e^{-(\lambda_S - w_A)t}\right) \cdot e^{\lambda_s t} \tag{31}$$

$$A(t) = \frac{P_1 DC}{(w_A - \lambda_S)} \cdot \left(e^{w_A t} - e^{\lambda_s t}\right) \tag{32}$$

Finally, by substitution $\lambda_S = w_S - \lambda_1^2 D$

$$A(t) = \frac{P_1 DC}{(w_A - w_S + \lambda_1^2 D)} \cdot \left(e^{w_A t} - e^{w_S t - \lambda_1^2 D t}\right) \tag{33}$$

The number of A-cells grows by means of A-growth and S-type transition. Then, for each of two regimes, this value approaches.

1. In the growth-dominated regime $w_A >> (w_S - \lambda_1^2 D)$, $A(t) \sim \frac{P_1 D}{w_A} \cdot^{w_A t}$
2. In the transition-dominated regime $w_A << (w_S - \lambda_1^2 D)$, $A(t) \sim \frac{P_1 DC}{w_S - \lambda_1^2 D t} \cdot e^{w_S t - \lambda_1^2 D t}$.

6 Numerical solution

To solve kinetic equations numerucally we calculated $S(x,t)$ on a lattice grid spacing in time Δt and space h distance apart. We choose the interval step Δt so it satisfies stability condition $(2D\Delta t \ll h^2)$. So,the S_k is number of S-cell at the grid point k and A is number of cells at the adsorbing boader.

6.1 In the bulk

$$\frac{\partial}{\partial t} S(x,t) = w_S S(x,t) + D \frac{\partial^2}{\partial x^2} S(x,t) \tag{34}$$

Can be rewritten as

$$S_k(t + \Delta t) = \left(1 - \frac{2D\Delta t}{h^2}\right) \cdot S_k(t) + \frac{D\Delta t}{h^2} \cdot \Big(S_k(t) + S_{k-1}(t)\Big) + w_S \Delta t \cdot S_k(t) \tag{35}$$

6.2 At the adsorbing boundary $x = 0$

$$\begin{cases} S_1(t + \Delta t) = \left(1 - \dfrac{2D\Delta t}{h^2}\right) \cdot S_1(t) + \dfrac{D\Delta t}{h^2} \cdot \Big(S_2(t) + (1 - P_1 h) \cdot S_1(t)\Big) + w_S \Delta t \cdot S_1(t) \\ A(t + \Delta t) = A(t) + w_A \Delta t \cdot A(t) + \dfrac{2D\Delta t}{h^2} \cdot P_1 h \cdot S_1(t) \end{cases} \tag{36}$$

6.3 At the reflective boundary $x = L$

$$S_L(t+\Delta t) = \left(1 - \frac{2D\Delta t}{h^2}\right) \cdot S_L(t) + \frac{D\Delta t}{h^2} \cdot S_{L-1}(t) + w_S \Delta t \cdot S_L(t) \tag{37}$$

7 Model with revertants

$$\begin{cases} \frac{\partial}{\partial t} S(x,t) = w_S S(x,t) + D \frac{\partial^2}{\partial x^2} S(x,t) + w_{AS} A \delta(x) \\ \frac{\partial}{\partial t} A = w_A A + P_1 D \cdot S(0,t) - w_{AS} A \end{cases} \tag{38}$$

with boundary conditions

$$\begin{cases} D \frac{\partial}{\partial x} S(0,t) = P_1 D \cdot S(0,t), & \text{partially adsorbing boader} \\ \\ \frac{\partial}{\partial x} S(L,t) = 0, & \text{reflective boader} \end{cases} \tag{39}$$

where w_S is a grownth rate of the S-type, D is a diffusion coefficient, P_1 is a non-negative constant. At $P_1 = 1$, the boundary condition becomes absorbing $S(0,t) = 0$. At $P_1 = 0$, the boundary condition becomes reflective $\frac{\partial}{\partial x} S(0,t) = 0$. w_A is a growth rate of A-type, term $P_1 D \cdot S(0,t)$ is transition flux from S-type to A-type, w_{AS} is a rate of transition from A-type to the S-type. $\delta(x)$ shows that revertants appear at the interface boarder.

7.1 Bakward-propogation for numerical calculation

A-type

$$A^n - A^{n-1} = w_A A^n \Delta t + P_1 D S_1^n \Delta t - w_{AS} A^n \Delta t \tag{40}$$

$$A^n = \frac{A^{n-1} + P_1 D S_1^n \Delta t}{1 + w_{AS}\Delta t - w_A \Delta t} \tag{41}$$

System of linear equations

$$\begin{cases} (1 - w_A \Delta t + w_{AS}\Delta t) A^n - P_1 \Delta x F S_1^n = A^{n-1} & \text{a-type with reveltants} \\ -w_{AS}\Delta t A^n + (1 + 2F - F(1 - P_1 h) - w_S \Delta t) S_1^n - F S_2^n = S_1^{n-1} & \text{partially adsorbing boarder} \\ -F S_{i-1}^n + (1 + 2F - w_S \Delta t) S_i^n - F S_{i+1}^n = S_i^{n-1}, & \text{in the bulk} \\ \\ -F S_{N-1}^n + (1 + F - w_S \Delta t) S_N^n = S_N^{n-1} & \text{reflective boarder} \end{cases} \tag{42}$$