

27febbraio 2019  
Incontro del  
Gruppo di lavoro sui  
BIOFILM

Società dei Naturalisti in  
Napoli, via mezzocannone 8  
Ore 9.30

# Modelli Matematici per Biofilm Multispecie

B. D'Acunto

Università di Napoli "Federico II"

# 1 Mathematical modelling of multispecies biofilms

Essential mathematical variable and functions:

space  $\mathbf{x} = (x, y, z)$  and time  $t$

$n$  number of species within the biofilm

$X_i(\mathbf{x}, t)$  concentration of species  $i$

substrates  $S_j(\mathbf{x}, t)$ ,  $j = 1, \dots, m$

Continuum approach mass balance

$$\int_V \frac{\partial X_i}{\partial t} d\mathbf{x} = - \int_{\partial V} \mathbf{g}_i \cdot \mathbf{n} dS + \int_V r_{M,i} d\mathbf{x}, \quad i = 1, \dots, n,$$

$r_{M,i}$  growth rate

$\mathbf{g}_i = \mathbf{u}X_i$  biomass flux

$\mathbf{u}$  biomass velocity

$$\frac{\partial X_i}{\partial t} + \nabla \cdot (\mathbf{u}X_i) = r_{M,i}, \quad i = 1, \dots, n.$$

## 2 1D mathematical modelling

$$\frac{\partial}{\partial t} X_i(z, t) + \frac{\partial}{\partial z} (u(z, t) X_i(z, t)) = r_{M,i}, \quad i = 1, \dots, n.$$

Nonlinear hyperbolic partial differential equations on

$$D = \{0 \leq z \leq L(t), \quad 0 < t \leq T, \quad T > 0\}.$$

Biofilm thickness  $L(t)$  is unknown together with  $\mathbf{X} = (X_1, \dots, X_n)$  and the biomass velocity  $u(z, t)$ .

$r_{M,i}(\mathbf{X}, \mathbf{S})$  depends on  $\mathbf{X}$  and substrates  $\mathbf{S} = (S_1, \dots, S_m)$ .

Free boundary value problems. Volume fraction

$$\frac{\partial}{\partial t} f_i(z, t) + \frac{\partial}{\partial z} (u(z, t) f_i(z, t)) = R_{M,i}(\mathbf{f}, \mathbf{S}), \quad i = 1, \dots, n,$$

$$R_{M,i} = r_{M,i} / \rho_i, \quad \mathbf{f} = (f_1, \dots, f_n).$$

Equation for the unknown function  $u$

$$\frac{\partial u}{\partial z}(z, t) = \sum_{i=1}^n R_{M,i}, \quad 0 < z \leq L(t).$$

The substrate diffusion within the biofilm is governed by semi-linear parabolic partial differential equations

$$\frac{\partial S_j}{\partial t} - D_j \Delta S_j = r_{S,j}(\mathbf{X}, \mathbf{S}), \quad j = 1, \dots, m,$$

$r_{S,j}$  substrate conversion rate,  $D_j$  diffusion constant.

### 3 Characteristic coordinates

The characteristics lines, fig. 3.1, for the equations

$$\frac{\partial}{\partial t} f_i(z, t) + \frac{\partial}{\partial z} (u(z, t) f_i(z, t)) = R_{M,i}(\mathbf{f}, \mathbf{S}), \quad i = 1..n,$$

are the lines  $z = c(z_0, t)$  defined by the following differential initial value problem

$$\frac{\partial}{\partial t} c(z_0, t) = u(c(z_0, t), t), \quad c(z_0, 0) = z_0, \quad 0 \leq z_0 \leq L(t).$$

Let us evaluate equations on the characteristic lines

$$\frac{df_i}{dt}(c(z_0, t), t) = F_i(\mathbf{f}(c(z_0, t), t), \mathbf{S}(c(z_0, t), t)), \quad i = 1..n$$

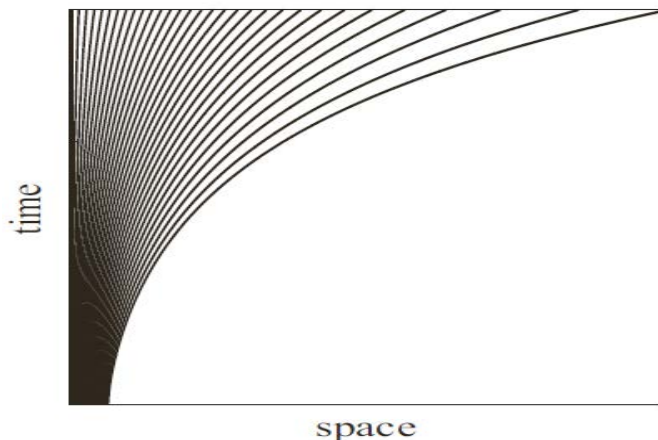


Figure 3.1: Characteristics

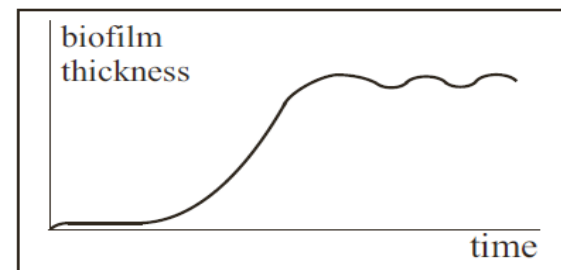


Figure 3.2: Typical diagram of biofilm growth

#### 4 Existence and uniqueness of solutions

#### 5 Invasion free boundary problem

Suppose the species of index  $k$  is initially nonzero only on a subinterval included in  $[0, L_0]$ . From Sec.4, it follows that  $f_k > 0$  on the space-time region delimited by the two characteristics starting from  $z_{0,1}$  and  $z_{0,2}$ , fig. 5.1, and it is  $f_k \equiv 0$  outside this region. In addition, consider

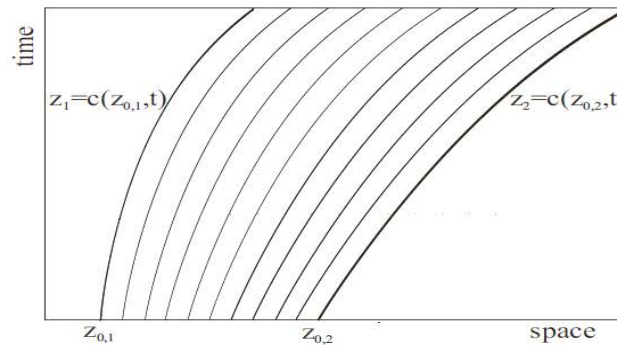


Figure 5.1: Space-time region where  $f_k > 0$ .

another species, say of index  $h \neq k$ , and assume that

$$f_{h,0}(z_0) = 0 \quad \forall z_0 \in [z_{0,1}, z_{0,2}].$$

From the reasonings above it follows that the species  $h$  cannot penetrate into  $D_k$ , since it is  $f_h = 0$  identically on  $D_k$ . In other words, a species cannot develop if it is not initially present within the biofilm.

This is an apparent limit of the model which is able to give positive answers in many situations, but it fails

in some others. It should be modified. A model capable to eliminate the problems is presented below. The presence of relatively large channels and pores within the biofilm matrix allows the entry of colonizing cells, present in the bulk liquid, and their establishment within the biofilm. According to these observations, in it is assumed that the diffusion of the colonizing bacteria is governed by a suitable new system of parabolic partial differential equations. A new term related to the invading bacterial species is added in the right-hand side of the equations that govern the biofilm growth.

$$\frac{\partial X_i}{\partial t} + \frac{\partial(uX_i)}{\partial z} = r_{i,M}(\mathbf{X}, \mathbf{S}) + \rho_i r_i(\boldsymbol{\psi}, \mathbf{S}), \quad i = 1, \dots, n,$$

where  $\psi_i(z, t)$  denotes the concentration of planktonic species diffusing from bulk liquid to biofilm and  $r_i(\boldsymbol{\psi}, \mathbf{S})$  the specific growth rate due to planktonic species,  $\boldsymbol{\psi} = (\psi_1, \dots, \psi_n)$ . The diffusion of the invading planktonic species through the biofilms is governed by the following system of parabolic partial differential equations

$$\frac{\partial \psi_i}{\partial t} - \frac{\partial}{\partial z} \left( D_{\psi,i} \frac{\partial \psi_i}{\partial z} \right) = r_{\psi,i}(\boldsymbol{\psi}, \mathbf{S}), \quad i = n_1 + 1, \dots, n,$$

where  $r_{\psi,i}(\boldsymbol{\psi}, \mathbf{S})$  denotes the conversion rate of motile planktonic species.

## 6 Attachment and detachment

The attachment biological process regards the biomass flux from the bulk liquid to the biofilm.

The opposite biomass flux, from the biofilm to the bulk liquid, is the detachment biological process.

Both processes strongly influence biofilm formation and growth. The attachment is important in the initial phase of biofilm formation, whereas the detachment is relevant for large mature biofilms.

Global mass balance for species  $i$  gives

$$A \frac{\partial}{\partial t} \int_0^{L(t)} X_i dz = A \rho_i \sigma_{a,i} - A \rho_i \sigma_{d,i} + A \rho_i \int_0^{L(t)} r_{M,i} dz,$$

$A$  constant sectional area

$\rho_i \sigma_{a,i}$  attachment flux for species  $i$

$\rho_i \sigma_{d,i}$  the detachment flux for species  $i$

Equation for the unknown function  $L(t)$  that describes the biofilm thickness

$$\dot{L}(t) = u(L(t), t) + \sigma_a - \sigma_d,$$

## 7 Initial phase of biofilm formation

$$\dot{L}(t) = u(L(t), t) + \sigma_a - \sigma_d.$$

When the detachment is the prevailing process, the inequality  $\sigma_a < \sigma_d$  implies that the free boundary velocity  $\dot{L}(t)$  is greater than the characteristic velocity  $u(L(t), t)$ , fig. 7.1 (left).

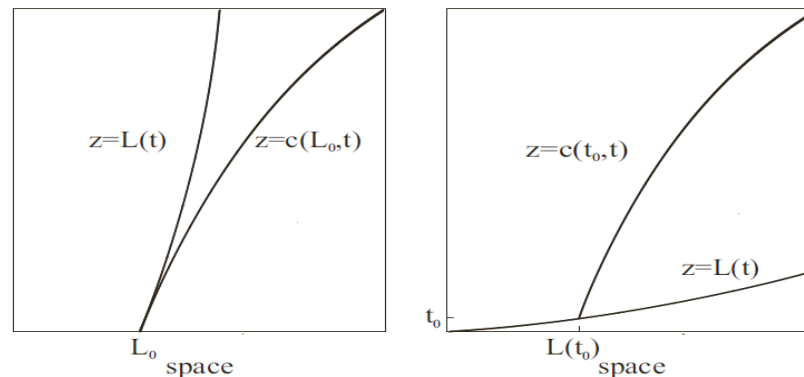


Figure 7.1:  $\sigma_a < \sigma_d$  (left);  $\sigma_a > \sigma_d$  (right)

When the attachment is the prevailing process, the inequality  $\sigma_a > \sigma_d$  implies that the free boundary velocity  $\dot{L}(t)$  is less than the characteristic velocity  $u(L(t), t)$ . The free boundary line is a space-like, fig. 7.1 (right). This situation occurs in the first times of biofilm formation when some bacterial species adhere to the support and a new colonization starts. From the mathematical point of view, an interesting feature is  $L(0) = 0$ .

## 8 Reactor free boundary problem

The mathematical modeling of a biofilm reactor usually takes into account two different compartments: the bulk liquid where the dissolved component concentrations vary according to the inlet and outlet flow and the flux into/from the biofilm, and the biofilm itself which grows and consumes the substrates provided by the bulk liquid. The two compartments are interconnected through a flux fig. 8.1.

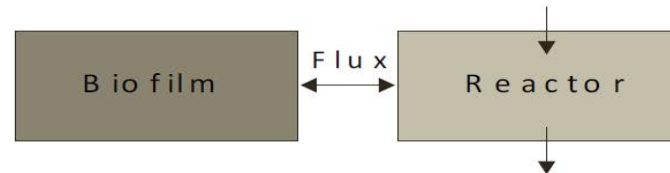


Figure 8.1: Biofilm reactor

Growth of bacterial species within the biofilm

$$\frac{\partial f_i}{\partial t} + \frac{\partial(uf_i)}{\partial z} = R_{M,i}(\mathbf{f}, \mathbf{S}), \quad i = 1, \dots, n.$$

Diffusion of substrates from reactor to biofilm

$$-D_j \frac{\partial^2 S_j}{\partial z^2} = r_{S,j}(\mathbf{X}, \mathbf{S}), \quad 0 < z < L(t), \quad j = 1, \dots, m,$$

with boundary conditions

$$\frac{\partial S_j}{\partial z}(0, t) = 0, \quad S_j(L(t), t) = S_j^*(t), \quad j = 1, \dots, m.$$

The functions  $S_j^*(t)$  satisfy the following initial value problems

$$V \dot{S}_j^* = Q(S_j^{\text{in}} - S_j^*(t)) - A D_j \frac{\partial S_j}{\partial z}(L(t), t), \quad S_j^*(0) = S_j^{\text{in}}, \quad j = 1, \dots, m,$$

where  $V$  denotes the reactor volume,  $Q$  flow rate through the reactor and  $A$  total biofilm area. All equations are mutually connected.

# Prospettive future