A novel model for biofilm growth and its resolution by using the hybrid immersed interface-level set method

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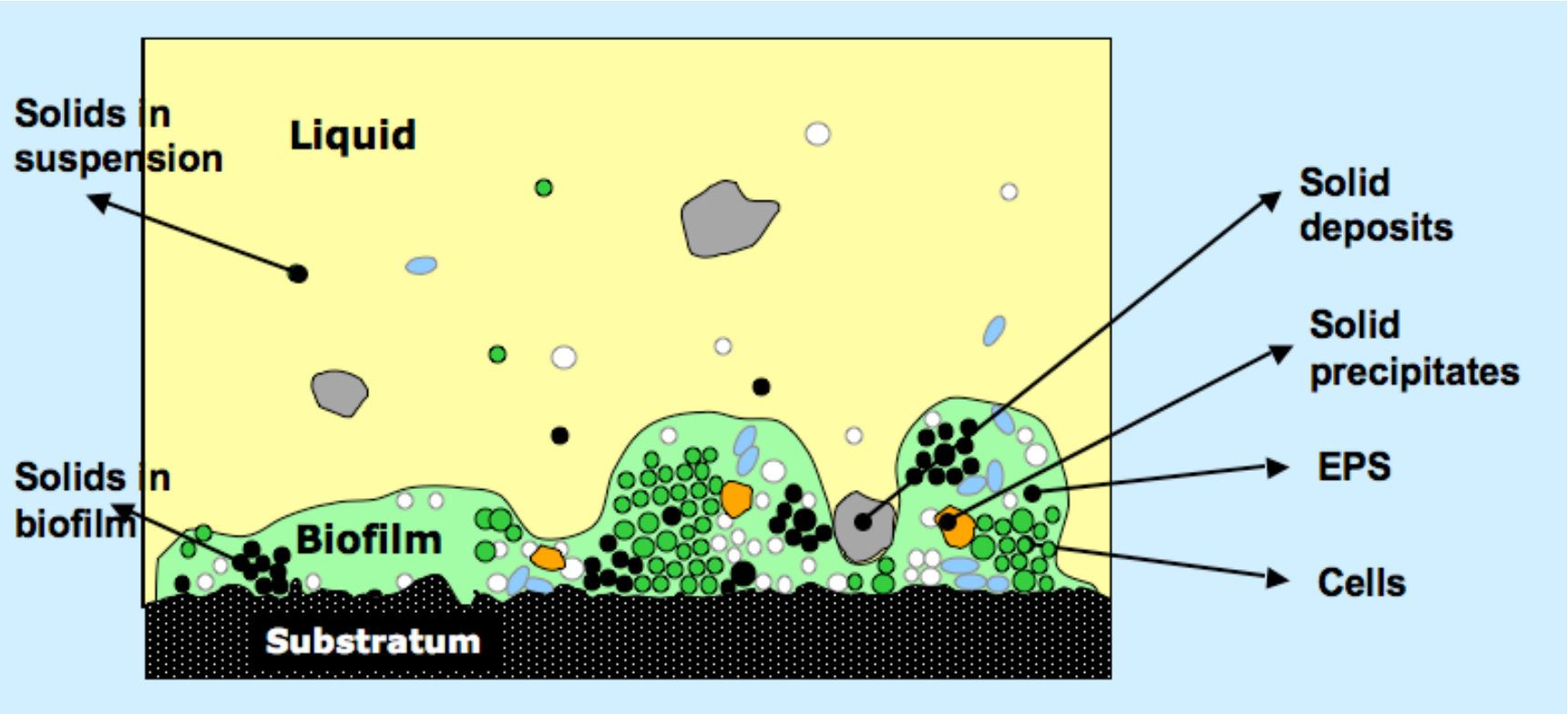
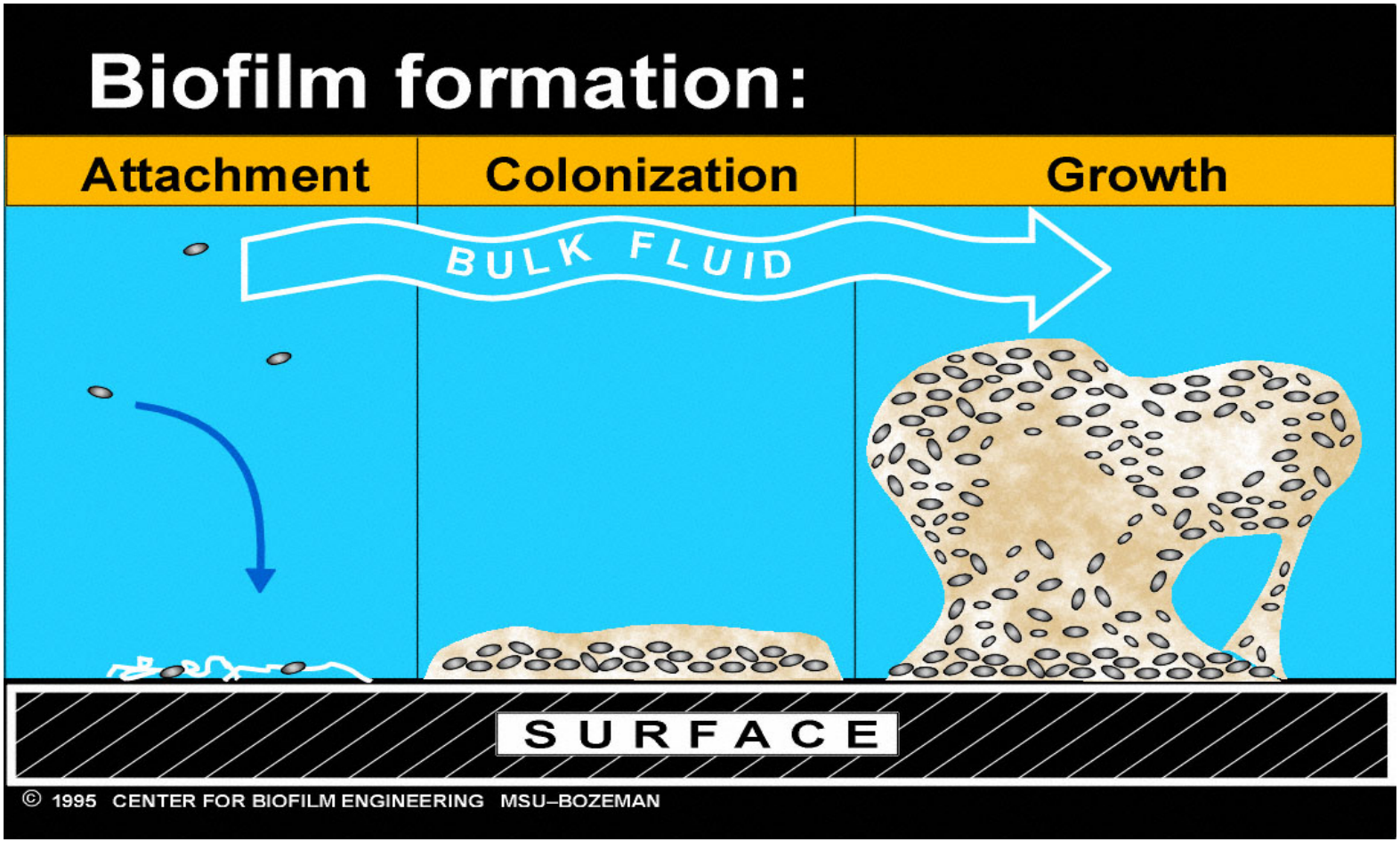
Congress Conca 60 - Workshop Chile-Euskadi
Basque Center for Applied Mathematics (BCAM) - Bilbao

What is a biofilm?



Biofilm formation



Why to study a biofilm?
Applications

- Bioremediation: technologies to assist the remediation of field sites contaminated with fuel hydrocarbons.
- Waste water treatment
- Bioleaching: A method to extract metals (such as copper) from the ore using only natural ingredients which are very easy to find in the environment: water, air and bacteria.

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Biofilm modeling
Generalities

Basic biofilm models are based upon three principles:

1. Transport mechanisms (advection, diffusion): for bringing nutrients into the biofilm.
2. Consumption and growing mechanisms.
3. Mechanisms for biofilm necrosis and loss.

New: Modeling of the *biofilm front* based on the Hele-Shaw flow (fingering instabilities).

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Modeling

Let $\Omega \subset \mathbb{R}^2$ be the rectangle $\Omega = (0, L_X) \times (0, L_Z)$, divided into two subregions: the biofilm compartment $z < h(x,t)$ and the liquid compartment $z > h(x,t)$, with curve interface $z = h(x,t)$ (the interface need not to be expressible as a function of x).

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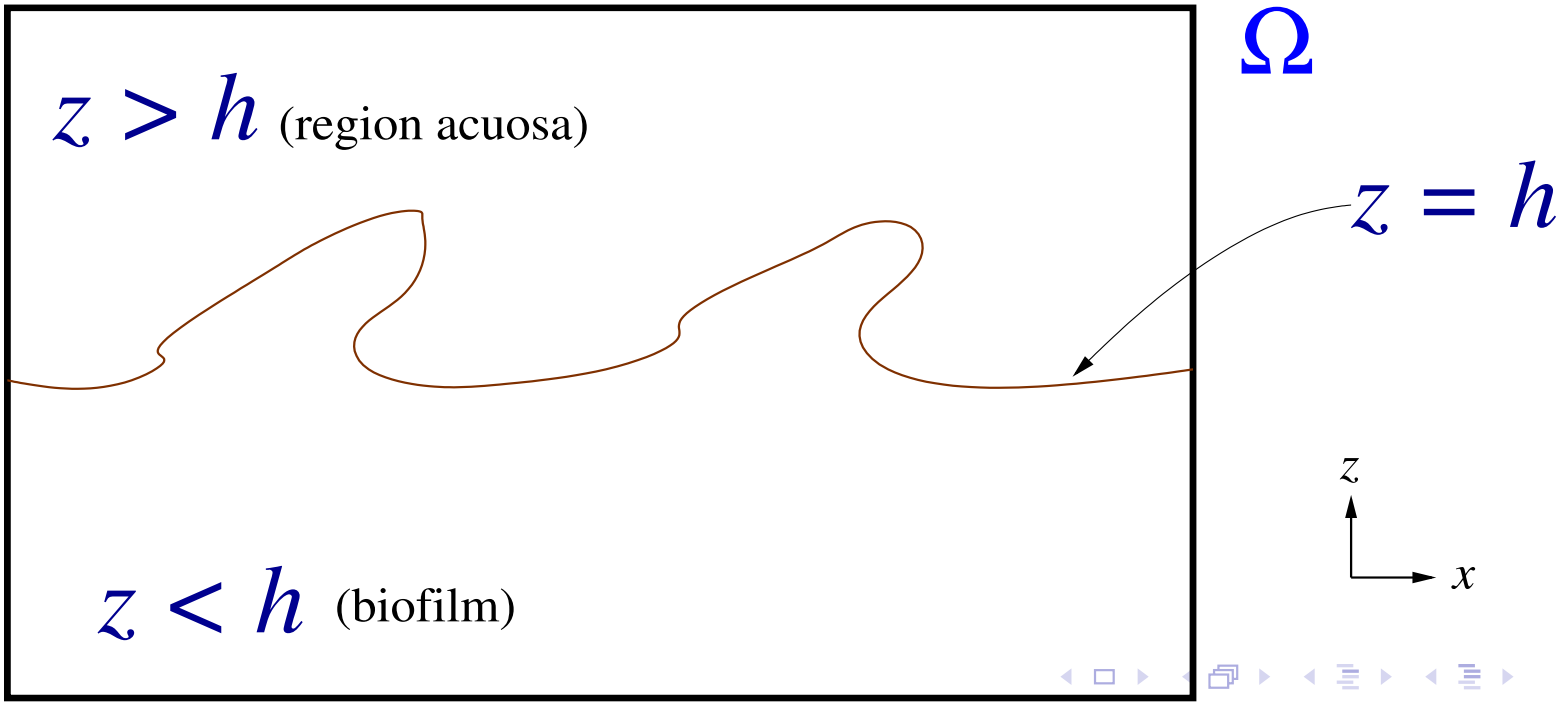

Hele-Shaw flow model

The biofilm is modeled as a homogeneous viscous fluid, which satisfies Darcy law

$$\mathbf{u} = -\nabla p$$

$\mathbf{u}$, p velocity and pressure resp. The biofilm may be growing or decaying, so that

$$\nabla \cdot \mathbf{u} = g \quad \text{in } \Omega_2(t)$$

for some g prescribed *growing function*. Note that g depends on the *substrate uptake rate* $U(S)$, i.e. $g = g(U)$, where S is a single limiting substrate (e.g., oxygen or glucose).

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The Hele-Shaw flow (revisited)

Pressure equations

$$-\nabla^2 p = \begin{cases} g(U) & \text{in the biofilm region,} \\ 0 & \text{in the liquid region.} \end{cases}$$

The transmissions conditions on the interface $\Gamma(t)$ are:

$$\begin{cases} [p] = d_0 \kappa & \text{(Laplace-Young condition)} \\ \left[\dfrac{\partial p}{\partial n}\right] = 0 & \text{(kinematic condition)} \end{cases}$$

d_0, κ are the *amalgamated surface tension coefficient* and the *mean curvature* resp.

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Substrate equations

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S_t + \nabla \cdot (S\mathbf{u}) - \frac{D_S T}{L_Z^2} \nabla^2 S &= 0 \quad \text{in } \Omega_1(t), \\
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Modeling of the substrate uptake rate function

Monod function

A typical choice for U is the *Monod* function

$$U(S) = \underbrace{\left(\frac{TU_m}{S_m}\right)}_{\nu} \delta_U (1+\mu) \frac{S}{S+K}$$

where T, U_m, S_m, μ, K are the *time scale of biofilm growth, reaction rate coefficient, maximum substrate concentration, maintenance coefficient* and *dimensionless half-saturation*, resp.

This form is also often used for the growing function g:

$$g(U(S)) = \frac{\nu S_m}{U_m} \delta_g \mu_m \left[(1+\mu) \frac{S}{S+K} - \mu \right]$$

Finally, δ_U and δ_g are scaling parameters.

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External boundary conditions

For the pressure:

$$\begin{cases} p|_{z=H} = 0, & \left.\dfrac{\partial p}{\partial z}\right|_{z=0} = 0, \\ p \text{ periodic in } x \text{ direction.} \end{cases}$$

For the substrate:

$$\begin{cases} S|_{z=H} = 1, & \left.\dfrac{\partial S}{\partial z}\right|_{z=0} = 0, \\ S \text{ periodic in } x \text{ direction.} \end{cases}$$

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The full biofilm model

Main difficulties

Key issue

Evolution of the biofilm front is a *unknown* of the model $\Rightarrow$ problem highly *non-linear*. We so deal with a *free boundary value problem*.

Generalized solutions

The presence of the interface implies that the solution is defined in a weak sense (it is discontinuous). Thus, well-posedness for this problem is a non-trivial issue.

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Numerical method for the interface evolution (1/3)

The level set method

Let $\phi(x, z, t)$ be satisfying $\phi(x, z, t) > 0$ for (x, z) in the liquid region and $\phi(x, z, t) < 0$ for (x, z) in the biofilm region. Then, by continuity $\phi(x, z, t)$ satisfies

$$(x, z) \in \text{ Biofilm front } \Leftrightarrow \phi(x, z, t) = 0.$$

Thus, the motion of the biofilm front is modeled by the *level set equation:*

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, & \text{for } (x, z) \in \Omega,\ t > 0, \\ \phi(x, z, 0) = \phi_0(x, z), & \text{for } (x, z) \in \Omega, \end{cases}$$

where $\phi_0(x, z)$ implicitly defines the initial biofilm front.

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The reinitialization process

In the level set method $\phi(x, z, t)$ corresponds to the signed normal distance from the point (x, z) to the interface $\Gamma(t)$. Although the level set equation transports the interface at the right velocity $\mathbf{u}$, it does not preserve ϕ as a distance function. To overcome this difficulty, we have used the reinitialization process:

$$\begin{cases} \psi_\tau + \mathrm{Sg}(\phi)(|\nabla\psi| - 1) = 0, \\ \psi(x, z, 0) = \phi(x, z, t), \end{cases}$$

where $\phi(x, z, t)$ corresponds to the level set function at time t_{n+1}, and $\mathrm{Sg}(\phi)$ is the one dimensional sign function composed with ϕ.

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Numerical method for the interface evolution (3/3)

Numerical methods for the level set equations

We apply this process every 15 time iterations, taking care of obtaining a steady state solution in order to numerically obtain that $|\nabla\psi| \approx 1$. The new function ψ has the same level sets as ϕ and is the signed normal distance to the interface.

Both Hamilton-Jacobi equations are solved by coupling a second-order TVD Runge-Kutta method to update ϕ (resp. ψ) from time t_n to t_{n+1} (resp. τ_n to τ_{n+1}), with a second-order ENO approximation to $\nabla\phi$ (resp. $\nabla\psi$). For an overview of the level set method see [Osher and Fedkiw, 2003].

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Numerical method for the pressure equations

Immersed Interface Method (IIM)

- The IIM [LeVeque and Li, 1994] deals with general interface conditions. This method is comparable, but more general than the immersed boundary method [Peskin, 1977].
- The discontinuities of the solution and/or coefficients are imposed in the standard method, by modifying it at *irregular grid points*, i.e., at grid points whose standard five-point stencil centered around it, is located in both sides of the interface (see figure in the next slide).
- If coefficients of the equation are continuous (which is our case), the IIM just adds a correction term in the right-hand side of the discretized equation at the irregular grid points.

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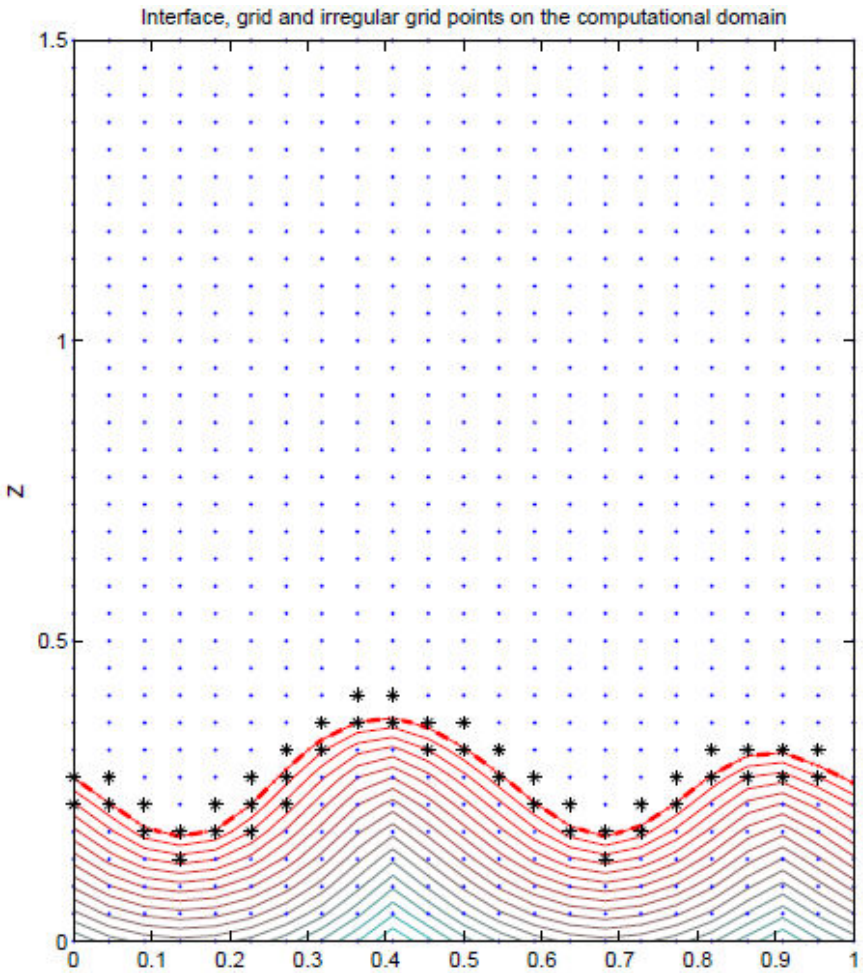
Immersed Interface Method

Interface (dashed line), regular grid (points) and irregular grid points (stars)



Algorithm

Step 1. $n \leftarrow 0$. Initialize the initial biofilm front, i.e., set $\phi(x, z, t = 0)$. At $t = 0$ the substrate is at its maximum level and uniformly distributed in the space, i.e. $S(x, z, t = 0) = 1$.

Step 2. Solve the pressure equations, and compute $\mathbf{u} = -\nabla p$ based on the IIM at time $t_n = n\Delta t$.

Step 3. Solve the substrate equations at time t_n.

Step 4. Update the position of the interface with the velocity field $\mathbf{u} = -\nabla p$, by solving the level-set equation. Reinitialize the level-set function every 15 time steps.

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Parameters

We have taken the following common parameters in our simulations [Picioreanu et al., 2000]:

Parameter	Symbol	Value	Units
Time scale of biofilm growth	T	1000	s
Monod half-saturation constant	K_S	$3.5 \cdot 10^{-4}$	kg m^{-3}
Diffusion coefficient	D_S	$2.3 \cdot 10^{-9}$	m^2 s^{-1}
Surface tension coefficient in water	γ	$72.8 \cdot 10^{-3}$	kg s^{-2}
Maximum specific growth rate	μ_m	$1.5 \cdot 10^{-5}$	s^{-1}

A key parameter is the ratio (maximum biomass growth rate)/(maximum internal transport rate of substrate) [Picioreanu et al., 1998b], which determines the biofilm heterogeneity. The growth ratio, G, is computed as $G = L_Z^2 U_m/(D_S S_m)$. By setting $S_m = 4$ and 100 mg/L, G is taken as 395 and 16. Moreover, U_m and d_0 are computed accordingly to these values.

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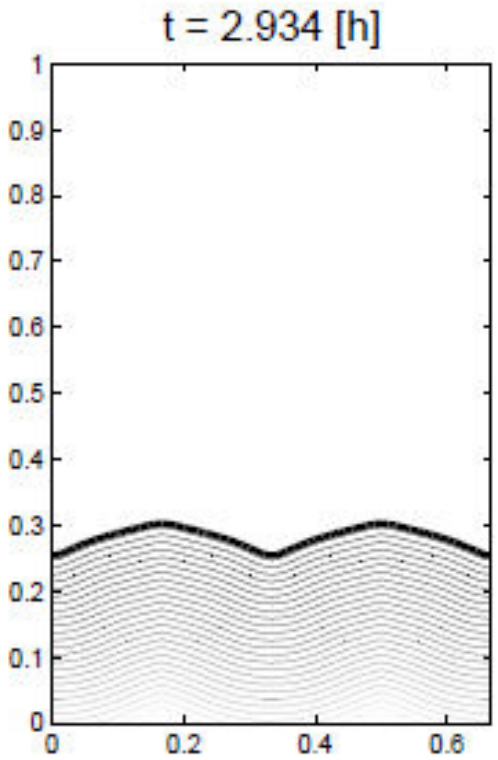
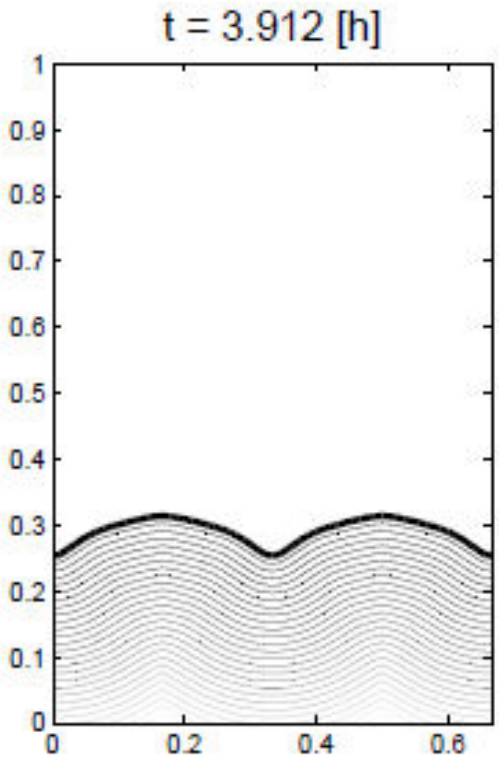
Numerical simulation for a transport-limited regime

Fingering formation





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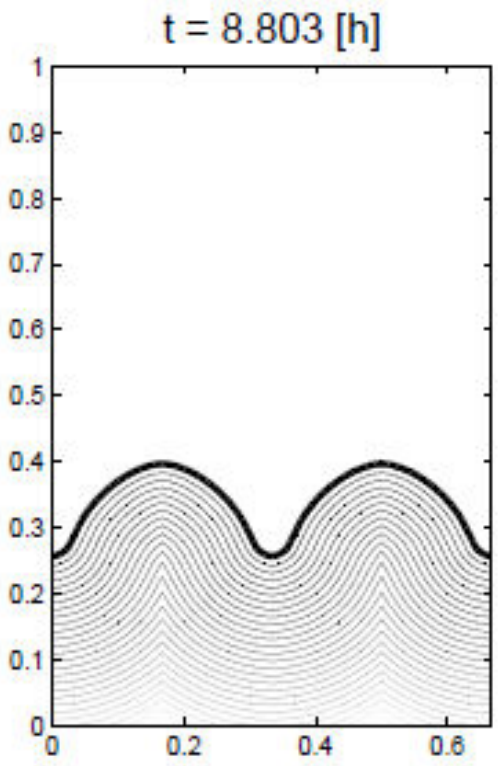
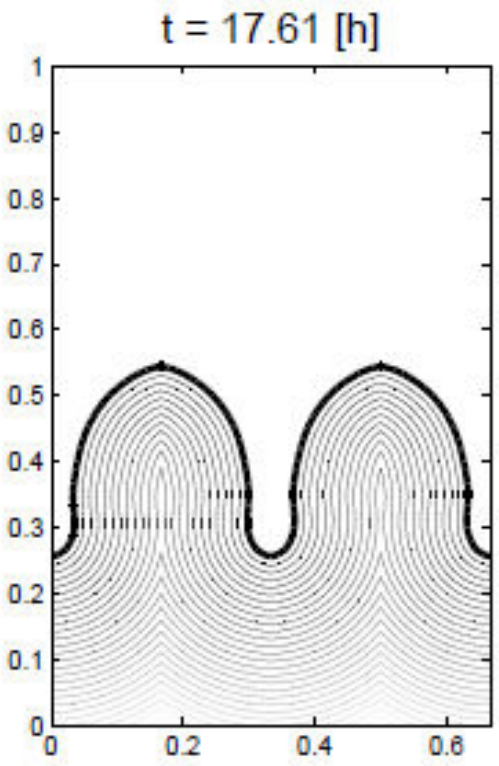
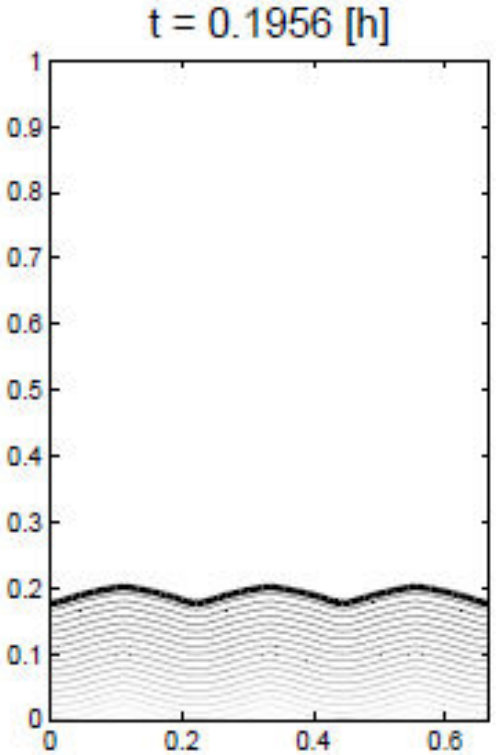
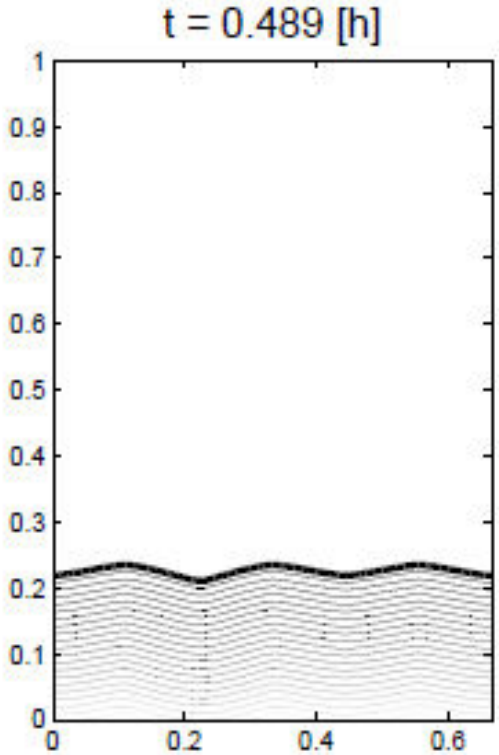




Numerical simulation for a growth-limited regime

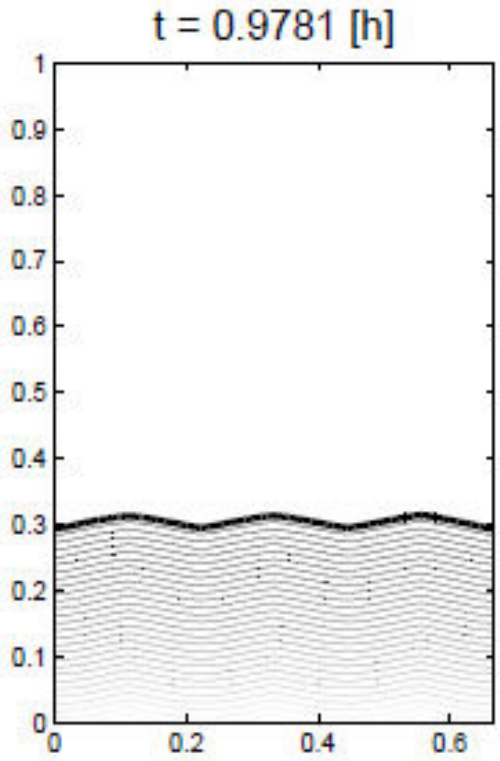
Compact-shaped biofilm

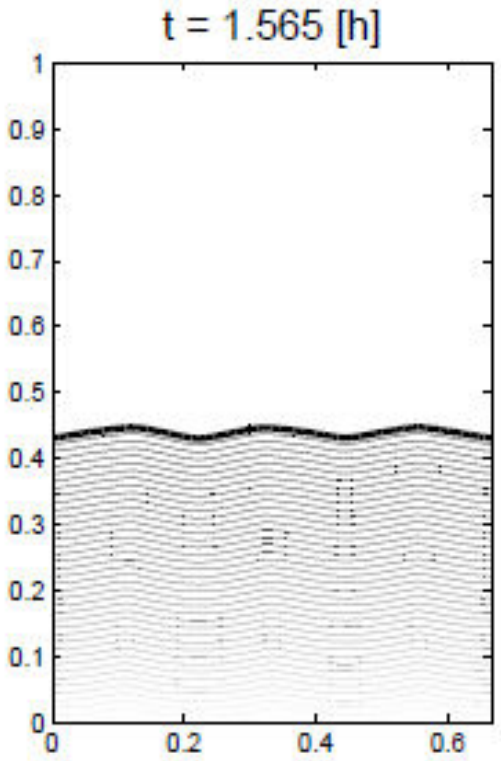




Numerical simulation for a growth-limited regime

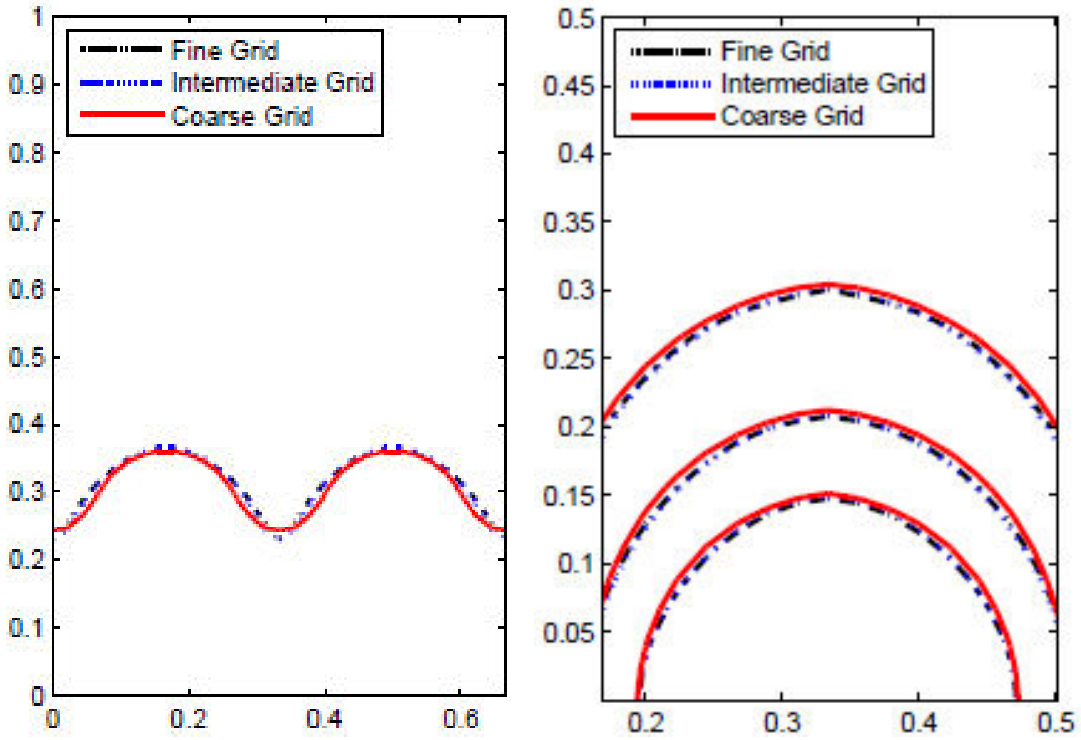
Compact-shaped biofilm





Grid refinement analysis

For two simulations



Conclusions

- Development of a new model that predict real biofilm behavior (finger-like, as well as, more compact structures, depending on the environmental conditions).
- Development of sophisticated numerical techniques (the IIM coupled to the level-set method) in order to evaluate the model.
- We could consider the flow field induced by the liquid and not only by the biofilm growth.
- We could consider two or more substrates as well as biofilm systems with multiple species.
- We could consider biofilm detachment, which also determines biofilm structure.
- In addition, we could consider that the fluid dynamics is governed by e.g. Navier-Stokes equations.

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Acknowledgments

This work was partially supported by Millennium Scientific Initiative under grant number ICM P05-001-F. The work of first author was also partially supported by Chilean Government Fondecyt-Conicyt Program under grant number 11080222 and by Universidad del Bío-Bío (grant DIUBB 121909 GI/C).

Thank you for your attention!!