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# Modelling of structural formation and growth of biofilms by a space-time meshfree collocation method

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**Résumé** — Une méthode de collocation espace-temps sans maillage est utilisée pour la modélisation des biofilms. Dans le modèle proposé, les biofilms sont représentés comme deux fluides incompressibles décrits par les équations de Stokes. Les exemples numériques démontrent le comportement typique des biofilms à savoir la formation de structures fongiformes en eau dormante.

**Mots clés** — biofilms, méthodes numériques sans maillage, formulation forte, spatio-temporelle, interpolating moving least squares.

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## 1 Biofilms

In environments where moisture, nutrient, and a surface are present, one will most probably also find biofilms, which may consist of one or different species of bacteria, archaeobacteria, algae as well as fungi or corrosion products. Biofilms can be found in 80% of all infections, e.g. infections of the urinary tract, catheter, and middle-ear, formation of dental plaque or sinusitis. A number of various models dealing with biofilms as a continuum has been proposed, e.g. [12, 8, 2]. We are interested in simulating the biofilm growth problem as a continuum without any probabilistic rules, applying a novel truly meshfree collocation method that uses a consistent discretization for both space and time.

## 2 A Space-Time Meshfree Collocation Method

The Space-Time Meshfree Collocation Method (STMCM) has been proposed by the first author for coupled problems on irregularly-shaped domains in [9]. In the following we apply the STMCM within a monolithic framework to a coupled problem of biofilm growth. Biofilm is modelled as a continuum using a two-biofluid representation governed by a system of incompressible Stokes equations and the moving interface is being implicitly tracked by solving the level-set equation. The presented technique is a truly meshfree method in both space and time which provides a straightforward and consistent way of solving partial differential equations in a monolithic setup.

### 3 A mathematical model of biofilm growth

The whole space-time domain of interest  $Q = \Omega \times I$ , where  $\Omega$  is the spatial part, and  $I = [0, T]$  the temporal one, consists of two parts :  $Q = Q^{a,i} = Q^a \cup Q^i$ , where  $Q^a$  is representing the biofilm itself – the *active* biofluid, and  $Q^i$  – representing the liquid substrate around – the *inactive* biofluid. In the proposed mathematical model the active biofluid is representing the biofilm and must model its behaviour, e.g. biofilm growth due to nutrients present in the domain, and the surrounding water, the inactive biofluid, is an auxiliary construction used for the solution strategy.

Fig. 1 shows the two subdomains  $\Omega_a$  and  $\Omega_i$  of the active and inactive biofluids, respectively, at some moment in time  $t = \text{const}$ . The interface  $\Sigma(t)$  at time  $t$  between  $\Omega_a$  and  $\Omega_i$  is described by a zero-level of a function  $\phi$ , which is chosen to be negative in the domain  $\Omega_a$  and positive in  $\Omega_i$ . The interface between the active and inactive biofluids is assumed to be sharp which agrees with the experimental observations, since the length scales of the problems under consideration are much larger in comparison with the transition area.

#### 3.1 Material description

In the proposed model the biofilm and the fluid around are considered to be incompressible fluids with different densities and viscosities. The unknowns to model the biofilm growth problem are :  $\vec{v}^a, \vec{v}^i$  – the velocity fields of the active and inactive biofluid respectively,  $p^a, p^i$  – the respective pressures of the biofluids, the level set function  $\phi$  which zero-level describes the interface between  $Q^a$  and  $Q^i$ , and the nutrient concentration  $n$  varying from zero to one.

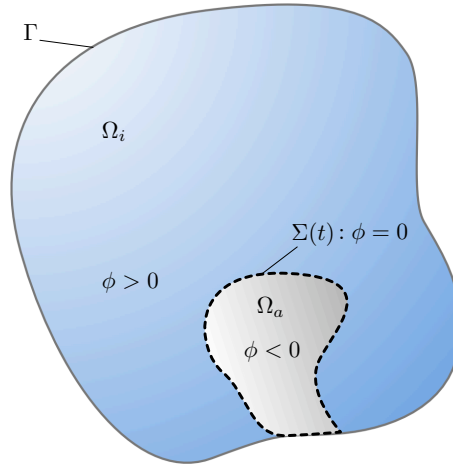


Fig. 1 – Biofilm growth model setup.

In process of a biofilm growth the fluid velocities are very slow and inertial forces are negligible compared to viscous forces. Hence, in the proposed model the set of incompressible Stokes equations governs the behaviour of biofluids, whereas equation (1) is the balance of momentum of the active and inactive biofluids. The incompressibility condition is given by equation (2) and the initial and boundary conditions are equations (3)-(4). The source term  $f_g$  in the equation (2) is important for the *growth* of the active biofluid and it will be defined later, and the inactive biofluid is not growing but rather flows out through the outer boundary  $\Gamma$ . The system of governing

equations reads as

$$-\operatorname{div} \mathbf{T}^{a,i} = \vec{0} \quad \text{in } Q^{a,i}, \quad (1)$$

$$\rho^{a,i} \operatorname{div} \vec{v}^{a,i} = f_g \quad \text{in } Q^{a,i}, \quad (2)$$

$$\vec{v}^{a,i}(\vec{x}, t = 0) = \vec{v}_0^{a,i} \quad \text{in } Q_{t=0}^{a,i}, \quad (3)$$

$$\vec{v}^{a,i}(\vec{x}) = \vec{v}^{a,i} \quad \text{on } \Gamma, \quad (4)$$

with the Cauchy stress tensor  $\mathbf{T}^{a,i} = -p^{a,i} \mathbf{I} + 2\mu^{a,i} \mathbf{D}^{a,i}$ , describing the inner stress state of the active and inactive biofluids, and the fluid kinematics with the strain rate tensor  $\mathbf{D}^{a,i} = \frac{1}{2}(\nabla \vec{v}^{a,i} + (\nabla \vec{v}^{a,i})^\top)$ . The assumed material model of the biofilm is a Newtonian fluid with linear dependence between shear stresses and strain rate represented by the kinematic viscosity  $\mu^{a,i}$ . The stress state of a biofluid at rest is defined by the hydrostatic pressure  $p^{a,i}$ . For an incompressible Newtonian fluid the equation (1) reads as

$$-\mu \nabla^2 \vec{v}^{a,i} + \nabla p^{a,i} = 0. \quad (5)$$

### 3.2 Nutrient description

Equation (6) is the advection-diffusion-reaction equation with a standard Monod reaction term  $f_c$  for nutrient *consumption* [7, 2, 3, 6] in the inactive biofluid only. In the active biofluid the nutrient of concentration  $n$  is consumed via the source term  $f_g$  in equation (2), which is responsible for the new biomass formation, i.e. the biofilm *growth*.

$$\frac{\partial n}{\partial t} + \vec{v}^{a,i} \cdot \nabla n - \nabla \cdot (d_n \nabla n) = f_c \quad \text{in } Q^{a,i}, \quad (6)$$

$$n(\vec{x}, t = 0) = n_0 \quad \text{in } Q_{t=0}^{a,i}, \quad (7)$$

where  $d_n$  is the diffusion coefficient. The nutrients are being convected, i.e. transported through the domain, by the flow velocity field  $\vec{v}^{a,i}$ .

### 3.3 Interface description

Various techniques exist on how to track moving interfaces [14, 10]. The level-set equation [14, 11] describes an evolution of a high-dimensional function  $\phi$ , and the zero-level of this function  $\phi$  is used for a description of a moving and deforming interface. The function  $\phi$  in the level-set equation is in most of the cases defined as a signed distance function from an arbitrary domain point to the interface. Thus, the different domains can be easily distinguished by simply looking at the sign of  $\phi$ . In the cases where the velocity is known at the interface only the velocity extension technique is used [1]. In our model this is not necessary, since the velocity field is defined in the whole domain. The level-set function  $\phi$  is chosen to be negative in the active biofluid domain  $\Omega_a$  and positive in the inactive biofluid  $\Omega_i$ , so that using the Heaviside function one can easily distinguish between the inactive and active biofluids in an implicit way and the material constants (densities and viscosities) are defined as follows

$$\rho^{a,i} = (1 - H(\phi)) \cdot \rho^a + H(\phi) \cdot \rho^i, \quad (8)$$

$$\mu^{a,i} = (1 - H(\phi)) \cdot \mu^a + H(\phi) \cdot \mu^i, \quad (9)$$

where  $\rho^a, \mu^a$  are respectively the density and kinematic viscosity of the active biofluid, and  $\rho^i, \mu^i$  – those of the inactive biofluid.

### 3.4 Nutrient consumption and biomass formation

The standard Monod terms for nutrient consumption  $f_c$  and growth  $f_g$ , respectively, [7], which are made dependent on the level-set function  $\phi$  in order to ensure that the nutrient is consumed in the active biofluid only, read as

$$f_c(\phi) = -(1 - H(\phi)) \cdot \gamma_n \frac{n}{\eta_n + n} = -f_g(\phi), \quad (10)$$

with  $\gamma_n$  – specific growth rate,  $\eta_n$  – Monod reaction coefficient. Parameters of the model used in the following validation example are given in Table 1.

Tableau 1 – Parameters used for simulations of biofilm growth.

Parameter	Symbol	Units	Value	Source
Specific growth rate	$\gamma_n$	$s^{-1}$	0.417	[13]
Monod reaction coefficient	$\eta_n$	$mg \cdot l^{-1}$	0.100	[13]
Nutrient diffusion coefficient	$d_n$	$m^2 \cdot s^{-1}$	9.67e-06	[13]
Ratio of viscosities	$\mu^a / \mu^i$	–	$1 \div 1000$	[4]
Ratio of densities	$\rho^a / \rho^i$	–	$1 \div 10$	assumed

### 3.5 An anisotropic biofilm growth in a channel

An anisotropic biofilm growth of several colonies in a channel with in- and outflow is modelled as shown in Fig. 2, on the channel walls non-slip conditions are implied. If the inactive biofluid is a stagnant one, the nutrient is not transported with the flow, but is diffused and consumed by the active biofluid, i.e. the biofilm, as in the previous example. Furthermore, we consider two configurations where individual colonies are located initially near to or far from to each other.

We note that in stagnant waters the biofilm tends to build mushroom- or finger-like structures. This observation is consistent with other reports, see e.g. [15, 5]. As long as nutrient is available in the whole system, the biofilm grows in all directions. However, with growing biomass the larger colonies start to dominate over the smaller ones due to their higher nutrient consumption and mushroom-like structures develop. The STMCM solution of the anisotropic biofilm growth example with several individual colonies located near to each other demonstrating the formation of mushroom-like structures is presented in Fig. 3.

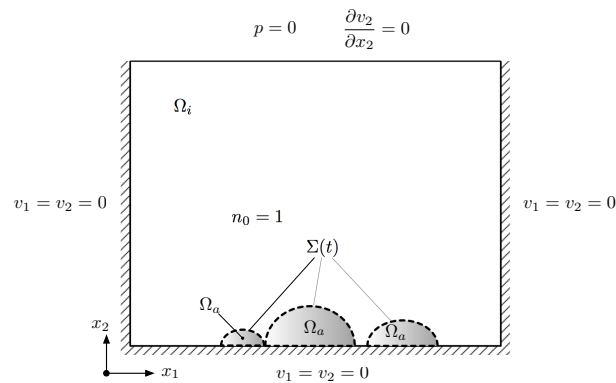


Fig. 2 – An anisotropic biofilm growth of several colonies in a stagnant fluid.

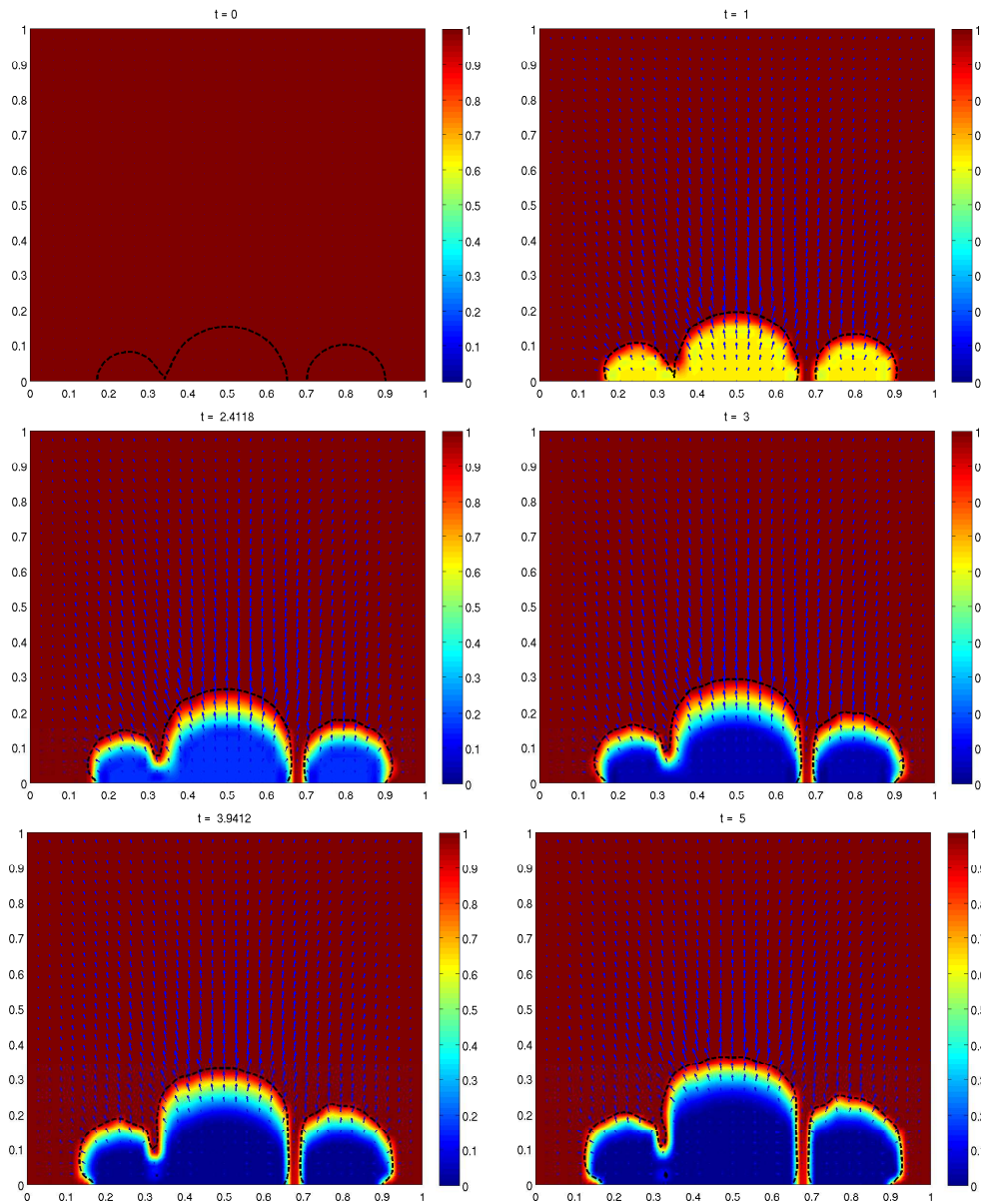


Fig. 3 – STMCM solution of the anisotropic biofilm growth example in a stagnant fluid : : formation of mushroom-like structures.

Depending on parameters, the behaviour of biofilm growth processes might be different. Individual biofilm colonies might remain isolated and grow upwards, as it was shown by the STMCM solutions. Such a behaviour is observed for higher values of the specific growth rate  $\gamma_n$  and low values of the nutrient diffusion coefficient, see e.g. [5, 7]. For smaller values of  $\gamma_n$ , however, the biofilms also move horizontally so that the colonies merge, see e.g. [7].

In order the presented model be used to simulate this kind of behaviour, certain rules for applying slip conditions at the channel walls must be incorporated, allowing tangential movement at the wall.

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