Advanced numerical schemes for the simulation of complex ecosystems

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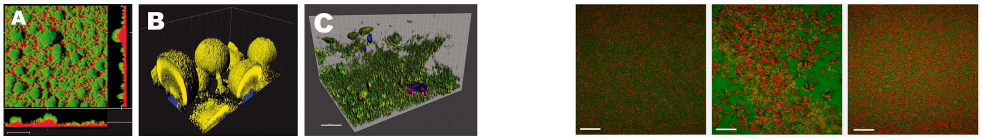
1 Context

There are many physical cases of flows composed of different gas or liquids interacting together. For example, tissue bodies and tumors can be described as a set of interacting viscoelastic materials. Powder-snow avalanches can be described as a mixture of fluid phases. Similarly, the rheology of the gut microbiota and its interactions with chyme (a mixture of partially digested food and water) and the host can be modelled using mixture theory [6]. Complex flows can also be found in many engineering application involving multiphase systems such as boiling water in nuclear reactors. Therefore, the framework of mixture theory is a common tool to model and study complex systems.

Mixture flows being ubiquitous in biophysics and engineering, the numerical schemes elaborated in the project will not be restricted to this specific application. Mathematical models based on mixture theory take the form of systems of partial derivative equations, coupled with algebraic constraints. The theoretical analysis of such systems and the characterization of the qualitative properties of the solutions is extremely complicated. Thus, it is important to develop efficient numerical methods able to accurately capture the solutions.

In this project, we are interested in applications of mixture models for describing biofilm dynamics. Indeed, mixture theory revealed a powerful approach to represent microbial biofilms where a consortium of cells is embedded in a polymeric structure [3, 8, 9]. Figure 1 present biofilms at microscopic scale.



(a) Bacterial biofilm image from [1]

(b) Micro-algae biofilm image from [5]

Figure 1: Example microscopy imaging of bacterial and micro-algae biofilms

In mixture theory, the unknowns of the model are requested to satisfy certain constraints. As far as the continuous equations are considered, several equivalent formulations of these constraints can be derived and

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used to bring out properties of the model. However, the preservation of these constraints by a numerical scheme is a challenge and, once a discretization set up has been adopted, it is not clear that all the formulations of the constraints remain equivalent. This issue can induce a loss of stability and accuracy, and eventually a dramatic loss of key physical properties of the simulated flows.

The first objective of the project is to adapt and extend the numerical scheme proposed in [2] in order to preserve these constraints. Next, we wish: (i) to design a version of the scheme that reaches second order accuracy in time and space, (ii) to explore and compare different modeling options.

The developments will be tested and illustrated with a multiphasic model representing the development of a photosynthetic biofilm, with application for biofuel, protein or drug production.

2 Mixture theory model for biofilms

2.1 Model description

We focus on a simplified 1D model for biofilms. Biofilms are made of microorganisms $\mathcal{A}$ (micro-algae or bacteria) and an extra-cellular matrix $\mathcal{E}$, immersed in water $\mathcal{L}$. Each component $k \in \{\mathcal{A}, \mathcal{E}, \mathcal{L}\}$ is described through macroscopic variables: the mass density ρ_k, the volume fraction ϕ_k which represents the percentage of volume occupied by the component k in an elementary piece of volume, and finally the velocity v_k. Therefore, by definition, the volume fractions satisfy at any time the volume filling constraint

$$\sum_{k \in \{\mathcal{A}, \mathcal{E}, \mathcal{L}\}} \phi_k = 1 \iff \phi_{\mathcal{A}} + \phi_{\mathcal{E}} + \phi_{\mathcal{L}} = 1. \tag{1}$$

It means that all the domain is filled and there is no vacuum. The local composition of the mixture evolves due to mechanical mechanisms such as transport and chemical reactions: several components react together leading to the consumption of some and the production of others. We denote by Γ_k the source term corresponding to the gain/loss of mass for the kth phase and the mass balance equations take the form

$$\partial_t(\rho_k \phi_k) + \partial_x(\rho_k \phi_k v_k) = \Gamma_k, \qquad k \in \{\mathcal{A}, \mathcal{E}, \mathcal{L}\}. \tag{2}$$

In this context, the volumic mass density ρ_k can be assumed to be constant. Thus the mass balance equations are equivalent to $\partial_t \phi_k + \partial_x(\phi_k v_k) = \Gamma_k/\rho_k$. Then summing these equations for each phase leads to the pseudo incompressibility constraint:

$$\partial_x \left(\phi_{\mathcal{A}} v_{\mathcal{A}} + \phi_{\mathcal{E}} v_{\mathcal{E}} + \phi_{\mathcal{L}} v_{\mathcal{L}}\right) = \frac{\Gamma_{\mathcal{A}}}{\rho_{\mathcal{A}}} + \frac{\Gamma_{\mathcal{E}}}{\rho_{\mathcal{E}}} + \frac{\Gamma_{\mathcal{L}}}{\rho_{\mathcal{L}}} \tag{3}$$

For biofilms, there are various biological processes to be taken into account: growth, extra-cellular matrix excretion and death. These reactions are schematically represented in Table 1. The parameters η_k are pseudo stoichiometric coefficients that quantify how much a reactant or a product is consumed or produced when a reaction occurs. The functions ψ are the reaction rates. They describe the speed at which a reaction takes place as a function of the local composition of the mixture. Therefore, the source terms read as follows:

$$\Gamma_{\mathcal{A}} = \psi_g - \psi_e - \psi_d, \qquad \Gamma_{\mathcal{E}} = \psi_e + \eta_{\mathcal{E}} \psi_d, \qquad \Gamma_{\mathcal{L}} = (1 - \eta_{\mathcal{E}})\psi_d - \eta_{\mathcal{L}} \psi_g.$$

The growth is mainly induced by substrate ($\mathcal{S}$) assimilation and liquid ($\mathcal{L}$) absorption. However, in first approximation we assume that the substrate is in excess. Thus the growth rate ψ_g takes the form of $\psi_g = \mu_g \mathcal{A}\mathcal{L}$ where μ_g is the maximal growth rate. The extra-cellular matrix excretion ψ_e and the the death rate ψ_d are assumed to be proportional to the quantity of micro-algae, thus $\psi_e = \mu_e \mathcal{A}$ and $\psi_d = \mu_d \mathcal{A}$, respectively.

The movement of the different components depends on the local forces applied to the system. For each component, a momentum balance equation gathers these physical features. According to [3, 8, 9], let us consider the hydrostatic pressure P, the elastic tensor for the biofilm constituents (micro-algae and extra-cellular-matrix) $\nabla \pi_k$, and the friction between phases F and the momentum supply induced by mass exchanges $\Gamma_k \mathbf{v}_k$. The

	Bioreaction representation		
Name	reactant(s)	Rate	Product(s)
Growth	$\eta_\mathcal{L}\mathcal{L} + \eta_\mathcal{S}\mathcal{S}$	$\xrightarrow{\psi_g}$	$\mathcal{A}$
Excretion	$\mathcal{A}$	$\xrightarrow{\psi_e}$	$\mathcal{E}$
Death	$\mathcal{A}$	$\xrightarrow{\psi_d}$	$\eta_\mathcal{E}\mathcal{E} + (1-\eta_\mathcal{E})\mathcal{L}$

Table 1: Schematic representation of the biochemical reactions considered for a simplified model of biofilm growth.

viscous stress tensor reads $\tau = \mu_k\Big(\nabla v_k + {}^t\nabla v_k - \frac{2}{3}(\nabla \cdot v_k)\mathrm{Id}\Big)$. The phases are also subjected to a gravity force g. Eventually, in 1D the momentum equations write

$$\partial_t(\rho_k\phi_k v_k) + \partial_x\Big(\rho_k\phi_k v_k^2\Big) + \partial_x\pi_k = -\phi_k\partial_x P + \frac{4}{3}\partial_x\Big(\mu_k\partial_x v_k\Big) + F_k + \Gamma_k v_k + \phi_k\rho_k g, \quad k \in \{\mathcal{A}, \mathcal{E}, \mathcal{L}\}.$$

Let us now detail the expression of the elastic tensors and the friction forces. For the liquid the elastic force is negligible, namely $\pi_\mathcal{L} = 0$. For the micro-algae ($k = \mathcal{A}$) and the extra-cellular matrix ($k = \mathcal{E}$), we assume that the elastic tensor is defined as in [2]: $\pi_k = \gamma_k\frac{\phi_k^{\beta_k}}{\phi_k^\star - \phi_k}$. In this expression, the coefficient γ_k has the homogeneity of a pressure, the exponent satisfy $\beta_k > 1$ and $\phi_k^\star$ is the so-called close-packing volume fraction for the component. As in [2, 3, 8, 9] we assume that the friction forces are proportional to the relative velocity $F_k = \sum_{p\neq k} f_{k,p}(v_p - v_k)$ with $f_{k,p}$ constant parameters. However, there are evidences that this force may depend on the local composition of the mixture; the adaptation of this feature and its impact assessment is one of the aim of the project, see section 4.1.

The model is supplemented by boundary conditions. Let $\Omega = [0, L]$ be the domain and $\partial\Omega$ its boundary. In 1D the domain should correspond to a biofilm core drilling in the orthogonal axis of the support where the biofilm develops. The velocities at the bottom of the domain which corresponds to the surface on which the biofilm develops vanishes: $v_k(0) = 0,\ k \in \{\mathcal{A}, \mathcal{E}, \mathcal{L}\}$. However, the velocity on the top must satisfy a constraint induced by the incompressibility constraint (3). Indeed, the integration the over the whole domain of equation (3) combined with the null velocity at the bottom lead to

$$\big(\phi_\mathcal{A} v_\mathcal{A} + \phi_\mathcal{E} v_\mathcal{E} + \phi_\mathcal{L} v_\mathcal{L}\big)(x = L) = \int_0^L \left(\frac{\Gamma_\mathcal{A}}{\rho_\mathcal{A}} + \frac{\Gamma_\mathcal{E}}{\rho_\mathcal{E}} + \frac{\Gamma_\mathcal{L}}{\rho_\mathcal{L}}\right)dx$$

To enforce this condition, let assume that the top velocities are given by $v_k = \int_0^L\Big(\frac{\Gamma_\mathcal{A}}{\rho_\mathcal{A}} + \frac{\Gamma_\mathcal{E}}{\rho_\mathcal{E}} + \frac{\Gamma_\mathcal{L}}{\rho_\mathcal{L}}\Big)dx$.

2.2 Synthesis of model equations

The PDE system under consideration writes:

$$\phi_{\mathcal{A}} + \phi_{\mathcal{E}} + \phi_{\mathcal{L}} = 1, \tag{4a}$$

$$\partial_t \phi_{\mathcal{A}} + \partial_x (\phi_{\mathcal{A}} v_{\mathcal{A}}) = \frac{\Gamma_{\mathcal{A}}}{\rho_{\mathcal{A}}}, \tag{4b}$$

$$\partial_t \phi_{\mathcal{E}} + \partial_x (\phi_{\mathcal{E}} v_{\mathcal{E}}) = \frac{\Gamma_{\mathcal{E}}}{\rho_{\mathcal{E}}}, \tag{4c}$$

$$\partial_t \phi_{\mathcal{L}} + \partial_x (\phi_{\mathcal{L}} v_{\mathcal{L}}) = \frac{\Gamma_{\mathcal{L}}}{\rho_{\mathcal{L}}}, \tag{4d}$$

$$\partial_t (\rho_{\mathcal{A}} \phi_{\mathcal{A}} v_{\mathcal{A}}) + \partial_x \left(\rho_{\mathcal{A}} \phi_{\mathcal{A}} v_{\mathcal{A}}^2\right) + \partial_x \pi_{\mathcal{A}} = -\phi_{\mathcal{A}} \partial_x P + \frac{4}{3} \partial_x \left(\mu_{\mathcal{A}} \partial_x v_{\mathcal{A}}\right) + F_{\mathcal{A}} + \Gamma_{\mathcal{A}} v_{\mathcal{A}} + \phi_{\mathcal{A}} \rho_{\mathcal{A}} g, \tag{4e}$$

$$\partial_t (\rho_{\mathcal{E}} \phi_{\mathcal{E}} v_{\mathcal{E}}) + \partial_x \left(\rho_{\mathcal{E}} \phi_{\mathcal{E}} v_{\mathcal{E}}^2\right) + \partial_x \pi_{\mathcal{E}} = -\phi_{\mathcal{E}} \partial_x P + \frac{4}{3} \partial_x \left(\mu_{\mathcal{E}} \partial_x v_{\mathcal{E}}\right) + F_{\mathcal{E}} + \Gamma_{\mathcal{E}} v_{\mathcal{E}} + \phi_{\mathcal{E}} \rho_{\mathcal{E}} g, \tag{4f}$$

$$\partial_t (\rho_{\mathcal{L}} \phi_{\mathcal{L}} v_{\mathcal{L}}) + \partial_x \left(\rho_{\mathcal{L}} \phi_{\mathcal{L}} v_{\mathcal{L}}^2\right) = -\phi_{\mathcal{L}} \partial_x P + \frac{4}{3} \partial_x \left(\mu_{\mathcal{L}} \partial_x v_{\mathcal{L}}\right) + F_{\mathcal{L}} + \Gamma_{\mathcal{L}} v_{\mathcal{L}} + \phi_{\mathcal{L}} \rho_{\mathcal{L}} g, \tag{4g}$$

with

$$\Gamma_{\mathcal{A}} = \psi_g - \psi_e - \psi_d, \qquad \Gamma_{\mathcal{E}} = \psi_e + \eta_{\mathcal{E}} \psi_d, \qquad \Gamma_{\mathcal{L}} = (1 - \eta_{\mathcal{E}}) \psi_d - \eta_{\mathcal{L}} \psi_g, \tag{5a}$$

$$\psi_g = \mu_g \mathcal{A} \mathcal{L}, \qquad \psi_e = \mu_e \mathcal{A}, \qquad \psi_d = \mu_d \mathcal{A}, \tag{5b}$$

$$\pi_k = \gamma_k \frac{\phi_k^{\beta_k}}{\phi_k^\star - \phi_k}, \qquad k \in \{\mathcal{A}, \mathcal{E}\}, \tag{5c}$$

$$F_k = \sum_{p \neq k} f_{k,p} \left(v_p - v_k\right), \qquad k \in \{\mathcal{A}, \mathcal{E}, \mathcal{L}\}. \tag{5d}$$

Most of the parameters come from [9] or [2]. The micro-algae and the extra-cellular-matrix viscosity coefficient are taken from [7]. All the parameters values are gathered in table 2.

3 Numerical scheme: implementation and analysis

The pressure is an unknown which is implicitly defined, associated to the constraint (1). The key point of the method presented in [2] is to build a numerical scheme able to preserve the different formulations of the constraints at the discrete level. The method is based on a time splitting method, in the spirit of projection methods in incompressible fluid mechanics. In the first step, the whole system is updated neglecting the constraint. In the second step, the velocities are corrected by using the incompressibility constraint (3). However, the computation of the pressure uses the definition of the convection fluxes in order to handle the incompressibility constraint and to preserve the consistency of the scheme. In turn, this discrete equation becomes non-linear.

4 Project targets

4.1 First tasks

1. Develop from [2] a finite volume scheme for the 3-phases model, preserving the constraints of the model,
2. Implement the numerical scheme using Python,
3. Adapt the friction forces and in order to account the local composition of the mixture by changing the friction coefficient $f_{k,p}$ into a function of the local composition: $f_{f,p}\left(\phi_k \phi_p\right)^\alpha$ and then compare the results with the original mode.
4. Change the model for the elastic tensor into:

Symbol	Name	Value	Unit
μ_g	Micro-algae maximal growth rate	2	day^{-1}
μ_e	Micro-algae maximal ECM excretion rate	0.4	day^{-1}
μ_d	Micro-algae maximal death rate rate	0.2	day^{-1}
$\eta_{\mathcal{L}}$	Liquid pseudo stoichiometric coefficient for growth	0.96	$\varnothing$
$\eta_{\mathcal{S}}$	Substrate pseudo stoichiometric coefficient for growth	0.146	$\varnothing$
$\eta_{\mathcal{E}}$	Liquid pseudo stoichiometric coefficient for growth	0.90	$\varnothing$
$\phi^{\star}_{\mathcal{A}}$	Micro-algae close packing threshold	~ 0.75	$\varnothing$
$\gamma_{\mathcal{A}}$	Micro-algae viscoelastic tensor coefficient	$1.5 \cdot 10^{-7}$	$kg/m/day$
$\beta_{\mathcal{A}}$	Micro-algae viscoelastic tensor exponent	1	$\varnothing$
$\phi^{\star}_{\mathcal{E}}$	Extra-cellular matrix close packing threshold	~ 0.75	$\varnothing$
$\gamma_{\mathcal{E}}$	Extra-cellular matrix viscoelastic tensor coefficient	$1.5 \cdot 10^{-7}$	$kg/m/day$
$\beta_{\mathcal{E}}$	Extra-cellular matrix viscoelastic tensor exponent	1	$\varnothing$
$\rho_{\mathcal{A}}$	Micro-algae volumetric mass density	1050	kg/m^3
$\rho_{\mathcal{A}}$	Extra-cellular matrix volumetric mass density	1050	kg/m^3
$\rho_{\mathcal{L}}$	Liquid volumetric mass density	1020	kg/m^3
$\mu_{\mathcal{L}}$	Liquid viscosity	10^{-3}	$Pa \cdot s$
$\mu_{\mathcal{A}}$	Micro-algae viscosity	$[0.1, 10]$	$Pa \cdot s$
$\mu_{\mathcal{E}}$	Extra-cellular matrix viscosity	$[0.1, 10]$	$Pa \cdot s$

Table 2: Model parameters

(a) $\pi = \gamma\phi^{\beta}$ as [3, 8, 9] in and study its impact on solution dynamic and the CFL condition,

(b) $\pi = -\gamma\big(\ln(1-\phi) + \phi + \phi^2\big)$ as [4] in and study its impact on solution dynamic and the CFL condition.

4.2 Model extensions

4.2.1 Light absorption

The growth of the biofilm is mainly induced by photosynthesis. Therefore, it is relevant to include the effects of light for micro-algae biofilms. This can be incorporated in the model (see [3, 8, 9]) by changing the mathematical law for growth from $\psi_g = \mu_g \mathcal{A}\mathcal{L}$ into

$$\psi_g = \mu_g \mathcal{A}\mathcal{L}\frac{2(1+K_{\mathcal{I}})\mathcal{I}}{\mathcal{I}^2 + 2K_{\mathcal{I}}\mathcal{I} + 1}, \qquad \mathcal{I}(t,z) = \frac{\mathcal{I}_{surf}(t)}{\mathcal{I}_{opt}}\exp\left(-\int_z^{z_{surf}} \tau(1-\mathcal{L})dh\right)$$

where $K_{\mathcal{I}}$ is a parameter associated to Haldane's law for the impact of the rescaled light intensity $\mathcal{I}$. The rescaled light intensity $\mathcal{I}$ depends on the light intensity at the surface $\mathcal{I}_{surf}$, the optimal light intensity $\mathcal{I}_{opt}$ and the absorption rate of the biofilm τ

4.2.2 Substrate concentration dynamic

The substrate $\mathcal{S}$ is a dissolved component within the liquid phase. In addition to the transport by the phase it can also diffuse at a rate $D_{\mathcal{S}}$ within the phase. Therefore, the masse balance equations for a dissolved $c_{\mathcal{S}}$ within a phase ϕ_k writes:

$$\partial_t(\rho_{\mathcal{L}}\phi_{\mathcal{L}}c_{\mathcal{S}}) + \partial_x(\rho_{\mathcal{L}}\phi_{\mathcal{L}}c_{\mathcal{S}}v_{\mathcal{L}}) - \partial_x(\rho_{\mathcal{L}}\phi_{\mathcal{L}}D_{\mathcal{S}}\partial_x c_{\mathcal{S}}) = \Gamma_{\mathcal{S}}$$

Then the micro-algae growth can account for the local substrate availability using Monod law, see [9]. Thus, ψ_g becomes:

$$\psi_g = \mu_g \mathcal{A}\mathcal{L}\frac{2(1+K_{\mathcal{I}})\mathcal{I}}{\mathcal{I}^2 + 2K_{\mathcal{I}}\mathcal{I} + 1}\frac{\mathcal{S}}{K_{\mathcal{S}} + \mathcal{S}}, \qquad \mathcal{I}(t,z) = \frac{\mathcal{I}_{surf}(t)}{\mathcal{I}_{opt}}\exp\left(-\int_z^{z_{surf}} \tau(1-\mathcal{L})dh\right)$$

where K_S is the half-saturation constant for the substrates. The external substrate supply is obtained through boundary conditions by imposing $\mathcal{S}(L) = \mathcal{S}^\star$ where $\mathcal{S}^\star$ is a reference concentration. All the parameters values associated to this extension can be found in [9].

4.2.3 Inclusion of additionnal states

If time permits, another population (bacteria) will also be included together with other substrates such as oxygen or CO_2. Bacteria consume the EPS produced by microalgae to grow and use oxygen, while microalgae use the CO_2 for photosynthesis. A scheme for a more automatic implementation of additionnal state variables will be proposed.

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