Contribution ID: **120** Type: **Poster Presentation**

Particle methods for the dynamics of porous biofilms with heterogeneous rheology and its interaction with human lung epithelium

Tuesday, 23 May 2023 10:30 (1h 30m)

In this presentation we are interested in operational applications and new numerical approaches for modeling the heterogeneous mucus bio-film of human lungs for the monitoring of cystic fibrosis (CF) therapies. At an operational level, we aim at predicting whether a therapy has a significant impact of the mucociliary clearance or not, that is to say predicting the ability of the respiratory mucus to be functional, i.e. to move together with the motion of the surrounding cells. By opposition, a non-functional mucus will not move sufficiently to clear the lung wall from allergens, toxic agents, viruses, bacteria and their residual products (DNA filaments and altered mucoid elements).

In this biological configuration, the mucus is itself a porous media made of Newtonian periciliary fluid (PCL) and highly concentrated mucins produced by the goblet cells, whose motion in the mucus will allow a mixture between the mucins and the PCL leading by reaction to a polymerized mucus with a particular rheology. Among the rheological features such as visco-elasticity, visco-plasticity, yield stress and shear-thinning, we focus on this last one which has been shown to be the dominant feature leading to non-functional mucus [3]. Moreover, the PCL is produced by the respiratory epithelium covering the lung membrane, another porous media that allows the transcytosis mechanism producing the PCL. Indeed, the PCL is not present or not working properly when the cystic fibrosis transmembrane conductance regulator protein CFTR presents a mutation responsible of CF.

The numerical simulation of such configurations has two main objectives. On the one hand, one can predict whether a mucus is functional or not, with respect to the rheological features that are measured from samples [4]. On the other hand, the numerical simulation allows to adjust the parameters of an upscaled model, including the mucus permeability and the tortuosity index that relates the effective diffusion and the molecular diffusion of chemical species by means of a power of the porosity.

The mucus mixing is modeled by $-div(2\mu(c,D)\,D(u)) = f - \nabla p$, the non-Newtonian stationary Stokes equation, where f is the driving force induced by the epithelial cell, μ is mucus viscosity, $D = (\nabla u + \nabla u^T)/2$ is the shear-rate of the velocity u, p is the pressure, and the incompressibility is satisfied by $div(u) = 0$. The mucin concentration $c(x,t)$ follows

$$\frac{\partial c}{\partial t} + div(uc) - div(\sigma \nabla(c)) = 0$$

and the shear-thinning rheology is driven by the relation

$$\mu(c,D) = \mu_\infty + (\mu_0(c) - \mu_\infty)\left(1 + 2\beta(c)^2|D|^2\right)^{\frac{q(c)-2}{2}}$$

which makes all these equations strongly coupled. We will show that the solutions of this system can be expressed by a Lagrangian formulation [1,2], called particle method, that the numerical result are compatible with clinical resume of the patients whose sputum rheology has been characterized [4], and that the upscaled tortuosity index can be carried out.

This work has been funded by French National Agency of Research, project MucoReaDy ANR-20-CE45-0022-01, and by Carnot Institute ISIFoR project MicroMineral P450902ISI.

Participation

In-Person

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Session Classification: Poster

Track Classification: (MS05) Biochemical processes and biofilms in porous media