Biofilm growth in porous media: derivation of a macroscopic model from the physics at the pore scale via homogenization

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ABSTRACT. This paper concerns the modelling of biofilm in porous media. A macroscopic model (at the Darcy's scale) is derived from the physics at the pore scale by using an upscaling technique, namely the homogenisation method of multiple scale expansions. The domain of validity of this macroscopic description depends on the order of magnitude of different dimensionless numbers arising from the description at the microscopic scale. We show that at the macroscopic scale (i) the flow is described by the classical Darcy's law (ii) the mass balance of the fluid includes a source term due to the biomass growth (iii) the transport of substrate is describe by a diffusion-advection-reaction equation (iv) the macroscopic biomass balance is given by a diffusion-reaction relation. The macroscopic reactive term is similar to the microscopic one. The homogenization process also shows that all the effective coefficients (permeability, effective diffusion tensors) arising in the macroscopic description depends on the biomass fraction. A simple example is presented.

1 INTRODUCTION

The study of biofilm in porous media spans a wide range of application going from environmental to medical applications. The growth of biofilm is a complex process that involves fluid flow, mass transport and biotransformation. Since more than two decades, a lot of work has been done in order to model biofilm development and morphology on planar or spherical substrata (Picioreanu *et al.,* 2003). In most of these works, the biofilm is viewed as a continuum, *i.e.* it is described by conservations equations law. In order to describe the behaviour of a bioreactor, it is not possible to simulate all the physical processes occurring at the pore scale by using the above models. To overcome these difficulties, a continuum approach (at the Darcy's scale) is usually preferred (Taylor *et al.*, 1990; Wood *et al.*, 2002). This approach consists in determining the continuous macroscopic description of the porous medium and it yields to the definition of average parameters (effective parameters). There are two ways of deriving this macroscopic description. The first one consists in deriving the macroscopic equivalent description at the macroscopic scale directly. The second one consists in deriving the continuous model starting from the description of the processes

at the microscopic scale (heterogeneities scale) by using an upscaling technique (Wood *et al.*, 2002).

This paper is aimed towards deriving the macroscopically equivalent medium from the description of the physical mechanisms at the microscopic scale using the homogenization method of multiple scale expansions for periodic structure (Bensoussan *et al.*, 1978; Sanchez-Palencia 1980). This method allows to obtain the macroscopic model without any prerequisite at the macroscale. The basic assumption of the method to be made is the existence of a Representative Elementary Volume (REV) of the medium, which is small in comparison to the macroscopic volume, *i.e.* with a good separation of scales: $\varepsilon = \lambda / L << 1$, in which λ and L are the characteristic lengths of the heterogeneities and of the macroscopic sample or excitation, respectively. Under these conditions, the macroscopic descriptions obtained are intrinsic of the geometry of the media and the phenomenon. They are also independent on the boundary conditions. In this study, we follow the approach suggested by Auriault (1991) which allows to derive different macroscopic descriptions in relation to the order of magnitude of the dimensionless parameters characterizing the phenomena. In this paper, this homogenization process is applied to a fluid saturated porous medium undergoing biofilm growth. The description at the microscopic scale and its dimensional analysis are presented in section 2.1 and 2.2, respectively. The macroscopic description is then presented in section 3.1. Finally, the influence of the biomass on the effective properties is discussed through a simple example (section 3.2).

2. MATERIALS AND METHODS

2.1 Description at the microscopic scale

We consider the flow of an incompressible Newtonian fluid through a periodic porous medium undergoing biofilm growth. In the following, we also assume that the porous medium is spatially periodic and consists of repeated unit cells (parallelepipeds), without lost of generality (Auriault, 1991). A period is shown in Figure 1.

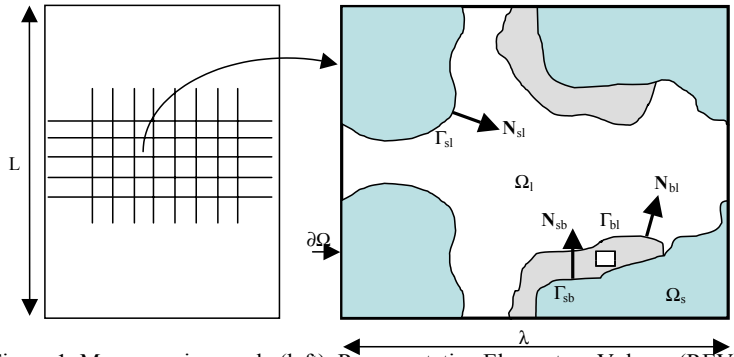

Figure 1. Macroscopic sample (left). Representative Elementary Volume (REV).

There are two characteristic length scales in this problem: the characteristic microscopic length scale λ of the pores and of the unit cell, and the macroscopic length L scale that may be represented by either the macroscopic pressure drop scale or by the sample size scale. For simplicity, we assume both macroscopic length scales to be of similar order of magnitude, O(L). Moreover we assume that the two length scales λ and L are well

separated: $\lambda << L$. The unit cell is denoted by □ and is bounded by $\partial\Omega$, the solid skeleton of the porous medium is denoted by Ω_s, the biofilm fixed on the solid skeleton is denoted by Ω_b, the bulk liquid phase of the unit cell is denoted by Ω_l, the solid-liquid interface inside the unit cell is Γ_{sl}, the solid-biofilm interface is Γ_{sb} and finally, the biofilm-liquid interface is Γ_{bl}. The porous medium is saturated, thus at any time t, we have: $f_s + f_b + f_l = 1$ where, $f_s = \Omega_s / \Omega$, $f_b = \Omega_b / \Omega$ and $f_l = \Omega_l / \Omega$ are the solid volume fraction, the biomass volume fraction and the fluid volume fraction within the Representative Elementary Volume, respectively.

In this study, the solid skeleton is assumed to be rigid. Thus the solid volume fraction f_s is constant. We also assume a steady-state slow flow. Consequently, the flow of an incompressible Newtonian fluid with constant physical properties within the liquid domain is described by the Stokes equation and the mass balance,

$$\mu\Delta\mathbf{v} - \nabla p = \mathbf{0} \quad \text{and} \quad \nabla\cdot\mathbf{v} = 0, \qquad \text{in}\,\Omega_l, \tag{1}$$

where $\mathbf{v}$ [m.s^{-1}] is the liquid velocity, p [Pa] is the liquid pressure and μ [Pa.s] is the constant dynamic viscosity. The biofilm is viewed as a continuous phase. For sake of simplicity, we consider only one limiting substrate. Biofilm detachment is neglected here (slow flow) but this phenomena could be taken into account by adding the correct terms in the equations and following the methodology presented below. The transport of the substrate in the bulk fluid follows the classical diffusion-advection equation,

$$\partial_t c_l + \mathbf{v}\cdot\nabla c_l - \nabla\cdot(D_l\nabla c_l) = 0 \qquad \text{in}\,\Omega_l, \tag{2}$$

where ∂_t is the temporal derivative, c_l [kg.m^{-3}] and D_l [m^2.s^{-1}] are the concentration of the substrate and the diffusion coefficient in the liquid phase respectively. In the biofilm phase the transport of the substrate is done by diffusion-reaction. The consumption of the nutrient by the microbes follows a Monods kinetics. Thus, we have

$$\partial_t c_b - \nabla\cdot(D_b\nabla c_b) + \frac{\mu_{max}}{Y}\frac{c_b c_x}{K + c_b} = 0 \qquad \text{in}\,\Omega_b, \tag{3}$$

where c_b [kg.m^{-3}] and D_b [m^2.s^{-1}] are the concentration of the substrate and the diffusion coefficient in the biofilm phase respectively, c_x [kg.m^{-3}] is the mass concentration of the biomass, μ_{max} [s^{-1}] is the maximum biomass growth rate, K [kg.m^{-3}] is the half-saturation constant and Y [kg.kg^{-1}] the yield rate of biomass from substrate. Finally, the mass balance of the solid phase in the biofilm is also described by a diffusion-reaction equation, in which the production rate of the solid cells is given by the Monods kinetics:

$$\partial_t c_x - \nabla\cdot(D_x\nabla c_x) - \mu_{max}\frac{c_b c_x}{K + c_b} = 0 \qquad \text{in}\,\Omega_b, \tag{4}$$

where D_x [m^2.s^{-1}] is the diffusion coefficient. To complete the pore-scale description we shall also consider the boundary conditions on Γ_{sl}, Γ_{bl} and Γ_{sb}. On Γ_{sl}, the liquid velocity verifies the adherence condition and the flux of substrate is equal to zero:

$$\mathbf{v} = \mathbf{0}, \qquad \text{on}\,\Gamma_{sl}, \tag{5}$$

$$-D_l\nabla c_l\cdot\mathbf{N}_{sl} = 0, \qquad \text{on}\,\Gamma_{sl}, \tag{6}$$

where $\mathbf{N}_{sl}$ is the unit outward normal of Γ_{sl}. On the interface Γ_{bl}, we have the continuity of tangential velocity, the continuity of mass and species fluxes,

$$\mathbf{v}\cdot\mathbf{T}_{bl} = 0, \qquad \text{on}\,\Gamma_{bl}, \tag{7}$$

$$(\rho_x\mathbf{w} - \rho\,(\mathbf{w}-\mathbf{v}))\cdot\mathbf{N}_{bl} = 0, \qquad \text{on}\,\Gamma_{bl}, \tag{8}$$

$$-D_x\nabla c_x\cdot\mathbf{N}_{bl} = 0, \qquad \text{on}\,\Gamma_{bl}, \tag{9}$$

$$(D_b\nabla c_b - D_l\nabla c_l)\cdot\mathbf{N}_{bl} = 0, \quad \text{and} \quad c_l = c_b, \qquad \text{on}\,\Gamma_{bl}, \tag{10}$$

where $\mathbf{T}_{bl}$ and $\mathbf{N}_{bl}$ are the tangential vector and the normal vector to the boundary Γ_{bl} respectively, $\mathbf{w}$ is the interface velocity, ρ_x [kg.m^{-3}] is the biomass density, ρ [kg.m^{-3}] is the fluid density. Finally, on Γ_{sb}, the fluxes of biomass and substrate are equal to zero,

$$-D_b \nabla c_b \cdot \mathbf{N}_{sb} = 0, \quad \text{and} \quad -D_x \nabla c_x \cdot \mathbf{N}_{sb} = 0, \quad \text{on } \Gamma_{sb}, \tag{11}$$

The set of equations (1) - (11) is the pore scale description.

2.2 Dimensional analysis

An important step of the homogenization process is the normalization of all equations describing physical processes at the pore scale. For that purpose, let us introduce in equations (1)-(11) the following representation of all dimensional variables:

$$\alpha = \alpha_c \, \alpha^*, \quad \text{with } \alpha = p, \mathbf{v}, \mu, c_l, D_l, c_b, D_b, t, c_x, D_x, \mu_{max}, Y, \mathbf{w}, \rho, \rho_x, \tag{12}$$

where the subscript 'c' and the superscript '*' denotes characteristic quantities (constant) and dimensionless variables respectively. In the similar way, the gradient operator is written $\nabla = \nabla^* / l_c$ where the characteristic length is l_c. The above pore scale description introduces eleven dimensionless numbers which characterize physical phenomena at the pore scale. These numbers are summarized in Table 1.

Table 1. Definition and estimation of the different dimensionless numbers.

Eq.	Dimensionless numbers	Physical phenomena	Order
(1)	$Q = O(p_c \, l_c / \mu_c \, v_c)$	Pressure force / viscous force	$O(\varepsilon^{-1})$
(2)	$P_l = O(l_c^2 / t_c \, D_{lc})$	Transient/diffusion transport of substrate in the fluid phase	$O(\varepsilon^2)$
(2)	$P_{el} = O(l_c \, v_c / D_{lc})$ (Péclet number)	Convective / diffusion transport of substrate in the fluid phase	$O(\varepsilon)$
(3)	$P_b = O(l_c^2 / t_c \, D_{bc})$	Transient/diffusion transport of substrate in the biofilm phase	$O(\varepsilon^2)$
(3)	$\phi^2 = O(\mu_{max\,c} \, c_{xc} \, l_c^2 / Y_c \, D_{bc} \, c_{bc})$ (Thiele number)	Consumption / diffusion transport of substrate in the biofilm phase	$O(\varepsilon^2)$
(3)	$C = O(K_c / c_{bc})$	Half saturation constant/concentration of substrate in the biofilm phase	O(1)
(4)	$P_x = O(l_c^2 / t_c \, D_{xc})$	Transient/diffusion transport of solid phase in the biofilm phase	$O(\varepsilon^2)$
(4)	$T_x = O(\mu_{max\,c} \, l_c^2 / D_{xc})$	Production/ diffusion transport solid phase in the biofilm phase	$O(\varepsilon^2)$
(8)	$R = O(\rho_{xc} / \rho_c)$	biomass density/ fluid density	O(1)
(8)	$M = O(v_c / w_c)$	fluid velocity/ interface velocity	$O(\varepsilon^{-1})$
(10)	$D = O(D_{lc} / D_{bc})$	Diffusion coefficient of the substrate in the liquid phase / biofilm phase	O(1)

According to the methodology presented in (Auriault, 1991), the next important step of the homogenization process consists in estimating these dimensionless numbers with respect to the parameter of scale separation ε. For sake of simplicity, we assume that the microscopic characteristic length $\lambda \approx 10^{-3}$ m (pore size) whereas the macroscopic characteristic length L=1 m (length of the bioreactor). Thus we have: $\varepsilon = \lambda / L \approx 10^{-3}$.

Moreover, we adopt the so called microscopic point of view (Auriault, 1991): $l_c = \lambda$ is used as the reference characteristic length to estimate the above dimensionless numbers. Now, dimensionless numbers can be estimated from characteristic values of physical properties ($\mu_c, D_{xc}, ..$) and physical phenomena ($v_c, p_c, ...$). It can be shown that the problem is homogenisable if $Q = O(\varepsilon^{-1})$ (Auriault, 1991) and if the interface velocity is small compared to the fluid velocity, *i.e.* $M = O(v_c / w_c) \geq O(\varepsilon^{-1})$ (Auriault, 1987). Moreover, we have $D_c \approx D_{lc} \approx D_{bc} \approx D_{xc} \approx 10^{-9}$ [$m^2.s^{-1}$]. Thus, $D = O(1)$ and $P_l \approx P_b \approx P_x = O(l_c^2 / t_c D_c)$. Assuming that the characteristic diffusion time of the process is $t_c \approx (L^2 / D_c)$, we get: $P_l \approx P_b \approx P_x = O(\varepsilon^2)$. The Péclet number P_{el} can take different orders of magnitude according to the intensity of the fluid flow. In this study we assume that $P_{el} = O(\varepsilon)$, *i.e.* there is no dispersion at the macroscopic scale. The Thiele number ϕ^2 may also take different order. Here, we assume that $\phi^2 = O(\varepsilon^2)$. The maximum biomass growth rate is the order of $10^{-5} s^{-1}$, thus we have typically $T_x = O(\varepsilon^2)$. The fluid density and the biomass density are the same order of magnitude: therefore $R = O(\rho_{xc} / \rho_c) = O(1)$. The half saturation constant is the same order of magnitude as the concentration of substrate within the biofilm. Thus, $C = O(K_c / c_{bc}) = O(1)$. Taking into account all of these estimations, the dimensionless microscopic description is written,

$$\mu^* \Delta^* \mathbf{v}^* - \varepsilon^{-1} \nabla^* p^* = \mathbf{0} \quad \text{and} \quad \nabla^* \cdot \mathbf{v}^* = 0, \qquad \text{in } \Omega_l^*, \qquad (13)$$

$$\varepsilon^2 \partial_{t^*} c_l^* + \varepsilon \mathbf{v}^* \cdot \nabla^* c_l^* - \nabla^* \cdot (D_l^* \nabla c_l^*) = 0 \qquad \text{in } \Omega_l^*, \qquad (14)$$

$$\varepsilon^2 \partial_{t^*} c_b^* - \nabla^* \cdot (D_b^* \nabla^* c_b^*) + \varepsilon^2 \frac{\mu_{max}^*}{Y^*} \frac{c_b^* c_x^*}{K^* + c_b^*} = 0 \qquad \text{in } \Omega_b^*, \qquad (15)$$

$$\varepsilon^2 \partial_{t^*} c_x^* - \nabla^* \cdot (D_x^* \nabla^* c_x^*) - \varepsilon^2 \mu_{max}^* \frac{c_b^* c_x^*}{K^* + c_b^*} = 0 \qquad \text{in } \Omega_b^*, \qquad (16)$$

$$\mathbf{v}^* = \mathbf{0}, \text{ and } -D_l^* \nabla^* c_l^* \cdot \mathbf{N}_{sl} = 0, \qquad \text{on } \Gamma_{sl}^*, \qquad (17)$$

$$\mathbf{v}^* \cdot \mathbf{T}_{bl} = 0, \quad (\rho_x^* \mathbf{w}^* - \rho^* (\mathbf{w}^* - \varepsilon^{-1} \mathbf{v}^*)) \cdot \mathbf{N}_{bl} = 0,$$
$$-D_x^* \nabla^* c_x^* \cdot \mathbf{N}_{bl} = 0, \quad (D_l^* \nabla^* c_l^* - D_b^* \nabla^* c_b^*) \cdot \mathbf{N}_{bl} = 0 \text{ and } c_l^* = c_b^*, \qquad \text{on } \Gamma_{bl}^*, \qquad (18)$$

$$-D_b^* \nabla^* c_b^* \cdot \mathbf{N}_{sb} = 0, \quad \text{and} \quad -D_x^* \nabla^* c_x^* \cdot \mathbf{N}_{sb} = 0, \qquad \text{on } \Gamma_{sb}^*, \qquad (19)$$

2.3 Upscaling

The next step is to introduce multiple-scale coordinates (Bensoussan *et al.*, 1978; Sanchez-Palencia, 1980). The two characteristic lengths L and λ introduce two dimensionless space variables: the macroscopic dimensionless space variable, $\mathbf{x} = \mathbf{X} / L$ and the microscopic dimensionless space variable, $\mathbf{y} = \mathbf{X} / \lambda$, where $\mathbf{X}$ is the physical space variable. Of course these two dimensionless space variables are linked through $\mathbf{x} = \varepsilon \mathbf{y}$. When using λ as the characteristic length, the dimensionless derivative operator becomes: $\nabla^* = \nabla_y + \varepsilon \nabla_x$, where the subscripts 'x' and 'y' denote the derivatives with respect to the variables $\mathbf{x}$ and $\mathbf{y}$, respectively. Following the multiple–scale expansion technique, the dimensionless unknowns $\varphi^* = p^*, \mathbf{v}^*, \mathbf{w}^*, c_l^*, c_b^*, c_x^*$ are sought in the form of asymptotic expansions of powers of φ,

$$\varphi^* = \varphi^{*(0)}(\mathbf{x}, \mathbf{y}) + \varepsilon \varphi^{*(1)}(\mathbf{x}, \mathbf{y}) + \varepsilon^2 \varphi^{*(2)}(\mathbf{x}, \mathbf{y}) + \ldots, \qquad (20)$$

where the corresponding basis functions $\varphi^{*(i)}$ are periodic functions or vectors with respect to space variable $\mathbf{y}$. Substituting these expansions in the set (13)-(19) gives by

identification of powers of φ, successive boundary-value problems to be investigated. Solving these problems leads to macroscopic description.

3 RESULTS AND DISCUSSION

3.1 Macroscopic description

The complete development for upscaling equations (13) - (19) will not be presented here. The mains results are the following:

- *macroscopic fluid flow*: at the first order of approximation, it can be shown that the fluid pressure is constant over the REV and the macroscopic fluid pressure gradient is acting as a driving force for the local flow,

$$p^{(0)} = p^{(0)}(\mathbf{x}), \qquad \mathbf{v}^{(0)}(\mathbf{x},\mathbf{y}) = -(\mathbf{k}(\mathbf{y})/\mu)\nabla p^{(0)} \tag{21}$$

where $\mathbf{k}(\mathbf{y})$ is the microscopic "permeability" tensor of the following boundary value problem over the REV,

$$\mu\Delta_y \mathbf{v}^{(0)} - \nabla_y p^{(1)} - \nabla p^{(0)} = \mathbf{0} \quad \text{and} \quad \nabla_y \cdot \mathbf{v}^{(0)} = 0, \qquad \text{in}\,\Omega_l\,, \tag{22}$$

$$\mathbf{v}^{(0)} = \mathbf{0}, \qquad \text{on}\ \Gamma_{sl}\ \text{and}\ \Gamma_{bl}\,. \tag{23}$$

The macroscopic fluid velocity which is obtained by volume averaging equation (21) gives us the Darcy's law. In dimensional form, we have

$$\left\langle \mathbf{v}^{(0)} \right\rangle = -\frac{\mathbf{K}}{\mu}.\nabla p^{(0)}, \quad \text{with} \quad \left\langle \mathbf{v}^{(0)} \right\rangle = \frac{1}{\Omega}\int_{\Omega_l} \mathbf{v}^{(0)}\,d\mathbf{y} \quad \text{and} \quad \mathbf{K} = \frac{1}{\Omega}\int_{\Omega_l} k(\mathbf{y})\,d\mathbf{y}\,, \tag{24}$$

where $\mathbf{K}$ [m^2] is the macroscopic permeability tensor of the porous medium. It can be shown that the dimensional macroscopic volume balance takes the form,

$$\nabla \cdot \left\langle \mathbf{v}^{(0)} \right\rangle + \left(\frac{\rho_x}{\rho} - 1 \right) \frac{\partial f_b}{\partial t} = 0 \tag{25}$$

where $f_b = \Omega_b / \Omega$ is the biofilm volume fraction. The first term and the second term of this equation are equal to the liquid flux and the expansion of the biofilm phase. Let us remark the presence of the second term in equation (25) depends on the order of magnitude of the dimensionless number M. If $M = O(v_c / w_c) \geq O(\varepsilon^{-2})$, *i.e.* the biofilm growth is very slow which is often the case in practical applications, this term is negligible and relation (25) reduces to $\nabla \cdot \left\langle \mathbf{v}^{(0)} \right\rangle = 0$.

- *macroscopic transport of substrate:* concerning the substrate, it can be shown that at the first other of approximation, the concentration of substrate is constant over the periodic cell, $c^{(0)}(\mathbf{x}) = c_l{}^{(0)}(\mathbf{x}) = c_b{}^{(0)}(\mathbf{x})$, and that the dimensional macroscopic transport equation for the substrate is written,

$$\phi \frac{\partial c^{(0)}}{\partial t} + \mathbf{v}^{\text{eff}} \cdot \nabla c^{(0)} - \nabla \cdot (\mathbf{D}^{\text{eff}} \nabla c^{(0)}) + f_b \frac{\mu_{max}}{Y} \frac{c^{(0)} c_x^{(0)}}{K + c^{(0)}} = 0\,, \tag{26}$$

where □ is the porosity of the porous medium without biofilm, $\mathbf{v}^{\text{eff}}$ and $\mathbf{D}^{\text{eff}}$ are the an effective velocity and the effective diffusion tensor, respectively. They are defined as follows,

$$\mathbf{v}^{\text{eff}} = \frac{1}{\Omega}\int_{\Omega_l} \mathbf{v}^{(0)} \left(\nabla_y \boldsymbol{\chi}_l + \boldsymbol{\delta} \right) dy\,, \tag{27}$$

$$\mathbf{D}^{\text{eff}} = \frac{1}{\Omega}\int_{\Omega_l} D_l \left(\nabla_y \boldsymbol{\chi}_l + \boldsymbol{\delta} \right) dy + \frac{1}{\Omega}\int_{\Omega_b} D_b \left(\nabla_y \boldsymbol{\chi}_b + \boldsymbol{\delta} \right) dy\,, \tag{28}$$

where $\boldsymbol{\delta}$ is the identity tensor, $\boldsymbol{\chi}_l(\mathbf{y})$ and $\boldsymbol{\chi}_b(\mathbf{y})$ are two $\mathbf{y}$-periodic vector fields solution of the following boundary value problem over the REV,

$$\nabla_y \cdot (D_l (\nabla_y \boldsymbol{\chi}_l + \boldsymbol{\delta})) = 0 \qquad \text{in } \Omega_l, \tag{29}$$

$$\nabla_y \cdot (D_b (\nabla_y \boldsymbol{\chi}_b + \boldsymbol{\delta})) = 0 \qquad \text{in } \Omega_b, \tag{30}$$

$$(D_b (\nabla_y \boldsymbol{\chi}_b + \boldsymbol{\delta}) - D_l (\nabla_y \boldsymbol{\chi}_l + \boldsymbol{\delta})) \cdot \mathbf{N}_{bl} = 0, \quad \text{and } \boldsymbol{\chi}_l = \boldsymbol{\chi}_b \quad \text{on } \Gamma_{bl}, \tag{31}$$

$$- D_l (\nabla_y \boldsymbol{\chi}_l + \boldsymbol{\delta}) \cdot \mathbf{N}_{sl} = 0, \qquad \text{on } \Gamma_{sl}, \tag{32}$$

$$\frac{1}{\Omega}\int_{\Omega_l} \boldsymbol{\chi}_l \, dy + \frac{1}{\Omega}\int_{\Omega_b} \boldsymbol{\chi}_b \, dy = 0. \tag{33}$$

At the macroscopic scale, the transport of substrate is described by a diffusion,-advection equation (26) including a consumption term.

- *macroscopic mass balance for the biofilm:* concerning the biofilm phase, it can be shown that at the first other of approximation, the mass concentration of the biomass is constant over the periodic cell, $c_x^{(0)} = c_x^{(0)}(\mathbf{x})$, and that the dimensional macroscopic mass balance is written,

$$f_b \frac{\partial c_x^{(0)}}{\partial t} - \nabla \cdot (\mathbf{D}_x^{eff} \nabla c^{(0)}) - f_b \frac{\mu_{max}}{Y} \frac{c^{(0)} c_x^{(0)}}{K + c^{(0)}} = 0, \tag{34}$$

where $\mathbf{D}_x^{eff}$ are the effective biomass diffusion tensor defined as follows,

$$\mathbf{D}_x^{eff} = \frac{1}{\Omega}\int_{\Omega_b} D_b (\nabla_y \boldsymbol{\beta}_b + \boldsymbol{\delta}) dy, \tag{35}$$

where $\boldsymbol{\beta}_b(\mathbf{y})$ is a $\mathbf{y}$-periodic vector field solution of the following boundary value problem over the REV,

$$\nabla_y \cdot (D_b (\nabla_y \boldsymbol{\beta}_b + \boldsymbol{\delta})) = 0 \qquad \text{in } \Omega_b, \tag{36}$$

$$D_b (\nabla_y \boldsymbol{\chi}_b + \boldsymbol{\delta}) \cdot \mathbf{N} = 0, \qquad \text{on } \Gamma_{sl} \text{ and on } \Gamma_{bl}, \tag{37}$$

$$\frac{1}{\Omega}\int_{\Omega_l} \boldsymbol{\chi}_l \, dy + \frac{1}{\Omega}\int_{\Omega_b} \boldsymbol{\chi}_b \, dy = 0. \tag{38}$$

At the macroscopic scale, the macroscopic mass balance is described by a diffusion-reaction equation (34) similar at the microscopic one (see Eq. (4)). .

3.2 Remarks

Relations (24), (25), (26) and (34) represent the macroscopic description for the fluid flow, the transport of the substrate and the biofilm growth in a porous medium. The macroscopic physical variables are the Darcy velocity $\langle \mathbf{v}^{(0)} \rangle$, the fluid pressure $p^{(0)}$, the concentration of the substrate $c^{(0)}$, the concentration of the biomass $c_x^{(0)}$ and the volume fraction of biomass $f_b = c_x^{(0)} / \rho_x$. The domain of validity of this macroscopic description depends on the order of magnitude of the dimensionless numbers presented in Table 1. This macroscopic description depends on three effective parameters: the permeability of the porous medium $\mathbf{K}$ [m^2], the effective diffusion tensor for the substrate $\mathbf{D}^{eff}$ [$m^2.s^{-1}$] and the effective biomass diffusion tensor $\mathbf{D}_x^{eff}$ [$m^2.s^{-1}$]. These effective parameters can be estimated through experiments or numerically by solving boundary value problems (22)-(23), (29)-(33) and (36)-(38) over the periodic cell. Obviously, these effective parameters depend on geometrical properties of the solid, liquid, and biofilm phases, and also on the physical properties at the microscopic scale. An analytical example is given in the next section.

3.3 Analytical example

Analytical results are of great interest because they permit us to point out general features concerning effective coefficients. Unfortunately, such results are available for only a few pore geometries. We investigate in this section porous media in which the pore system consists of parallel plane fissures, as shown in Figure 2. The initial pore thickness is denoted h and the initial porosity is $\phi = h/(h+e)$. The biofilm is assumed to be uniform on the solid phase and its thickness is denoted e_b. At any time, the fluid volume fraction and biomass solid fraction are defined as $f_l = (h-2e_b)/(h+e)$ and $f_b = 2e_b/(h+e)$ respectively. Solving boundary value problems (22)-(23), (29)-(33) and (36)-(38) over REV, it can be shown that in the plane ($\mathbf{e}_1$, $\mathbf{e}_2$),

$$\mathbf{K} = K\,\boldsymbol{\delta} \qquad \text{with } K = \frac{1}{12}(h-2e_b)^3 = \frac{1}{12}(h+e)^3(\phi - f_b)^3, \tag{39}$$

$$\mathbf{D}^{eff} = D^{eff}\,\boldsymbol{\delta} \qquad \text{with } D^{eff} = f_b D_b + f_l D_l = f_b D_b + (\phi - f_b) D_l, \tag{40}$$

$$\mathbf{D}_x^{eff} = D_x^{eff}\,\boldsymbol{\delta} \qquad \text{with } D_x^{eff} = f_b D_x \tag{41}$$

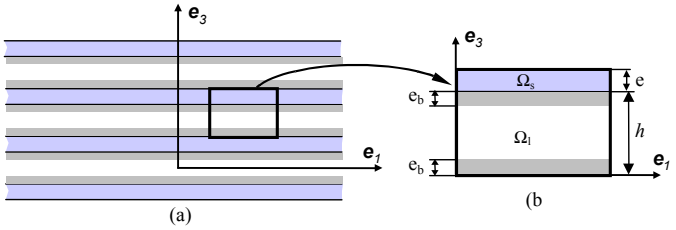

Figure 2. (a) Macroscopic sample. (b) Representative Elementary Volume (REV).

4 CONCLUSIONS

A macroscopic model describing biofilm processes in porous media has been derived by using a deterministic homogenization method. The domain of validity of this model is given by the order of magnitude of dimensionless numbers. The effective parameters arising in the macroscopic model depends on geometrical properties of the different phases, and the physical properties at the microscopic scale. A simple example was presented. Futher works concern the numerical estimation of the effective parameters for more complex geometries of porous media and the experimental validation of the macroscopic model. Some simulation results will be presented during the oral presentation

5 ACKNOWLEDGEMENTS

This work is part of a project entitled “Biofiltration des gaz”. Financial support of the whole project was provided by the “Ministère de la recherche et des Nouvelles Technologies” in collaboration with DGA, CNRS and INRS.

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