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Modelling on the effect of diffusive and convective substrate transport for biofilm

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ABSTRACT

A one-dimensional biofilm model was developed based on the basic principle of conservation of mass. Three simple, generic processes were combined in the model which includes microbial growth, diffusive and convective mass transport. The final model could generate a quantitative description of the relationship between the microbial growth and the consumption of substrate (oxygen) within the fixed biofilm thickness. Mass transfer resistance contributes large influence on the substrates and microbial concentration across the biofilm thickness due to the effect of biofilm structure.

1. Introduction: biofilms and their models

Biofilms are a common form of microbial ecosystems associated with surfaces. The ability of bacteria to attach to surfaces and form biofilms has becoming an important advantage over bacteria growing in suspension. Suspended bacteria is susceptible to water flow, but bacteria in biofilms are protected from washout can grow in locations where their food supply remains abundant. Biofilms growth is well recognized phenomenon in process industry. Biofilm accumulation may cause biological fouling, heat transfer losses, product quality deterioration and biocorrosion. On the metal surfaces, bacteriological growth may alter the microclimate locally such as by producing gradients in oxygen concentration or pH, excreting organic acids or allowing the proliferation of certain anaerobic bacteria within the biofilm.

Biofilm formation seems to be primarily dependent on the interaction between mass transport and conversion processes. Experimental research has shown that biofilms developed in a multitude of patterns [1,2]. Traditionally, development of biofilms is seen as the formation of a layered structure growing from the substratum. The use of one-dimensional biofilm models as described in [3,4] strengthened this view. All the property gradients like those of substrate concentration, biomass density, etc. in these models are one-dimensional, varying only in the direction from the bulk liquid to the carrier surface.

Better understanding of biofilm morphology is important not only for its characterization but also for describing the internal and external mass transfer resistances. The external mass transfer resistance is given by the thickness of the concentration boundary layer, which is directly correlated to the hydrodynamic boundary layer resulting from the flow pattern over the biofilm surface. On the one hand, the fluid flow drives the biofilm growth by regulating the concentration of substrates and products at the solid liquid interface and on the other hand, the flow shears the biofilm surface, eroding its structure. While the flow changes the biofilm surface, the interaction is reciprocal because a new biofilm shape leads to a different place of boundary condition, thus, produces different flow and concentration fields [5].

In most mechanistic biofilm models, transport of dissolved components in the biofilm is described by Fick's First Law with molecular diffusivities which are assumed to have no gradients. However, in recent experiments it has been demonstrated that spatial gradients of the diffusivity in the biofilm exist, together with the convective transport of the dissolved components [6]. This finding can have a significant influence on biofilm modelling. Besides diffusion, convection is also important for the overall mass transport through the biofilm. Experiment by DeBeer and Stoodley [7] have shown that the concentration boundary layer can be parallel to the substratum (at low flow velocity) but can also follow the biofilm shape (at higher flow velocity). The first case is analogous to the work of previous model of biofilm formation [8]. However, to model the later case requires calculation of the flow pattern around the biofilm surface. Modelling fluid flow will also eventually give the possibility of modelling the biofilm detachment due to liquid shear stress [9]. Recently, Picioreanu et al. [10] described the influence of convective transport on substrate conversion is geometrically heterogeneous biofilm structures. The first

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effort to explain biofilm heterogeneity with a 2-D model including hydrodynamic process, substrate transport by diffusion and convection, biomass growth and spreading is reported in Picioreanu et al. [9].

Modelling is a powerful tool to studying biofilm growth and its effects. Mathematical models come in many forms that can range from very simple empirical correlations to sophisticated and computationally intensive algorithms that describe 3-D biofilm morphology. The best choice depends on the type of biofilm system under investigation, the objectives of the model user, and the modeling capability of the user. In this work, we developed a simple model to link the substrate flux into the biofilm to the fundamental mechanisms of substrate utilization and mass transport. The models assumed the simplest possible geometry (a slab) and biomass distribution, which can capture the important phenomena of the substrate diffusion through the thickness of the biofilm.

2. Modelling aspects

2.1. Physical description

The final goal of this work is to build a model that can generate a quantitative description of the relationship between the microbial growth and consumption of substrate (oxygen) within fixed biofilm thickness. The model described in this article therefore includes: (1) liquid flow around the biofilm, (2) substrate mass transport by diffusion and convection in the liquid phase and by diffusion in the biofilm-gel matrix, and (3) substrate conversion and biomass growth. In the present literature, several aspects have been taken into account in constructing the biofilm models. The basic ones which were considered include diffusion, convection, reaction (substrate consumption and biomass production), biofilm growth and detachment.

The diffusion can be described by considering Fick's First Law while convection can be described by including the Navier–Stokes equations for fluid flow. The complication when using model that incorporates convective mass transport is that the fluid velocity must either be known or calculated before hand, which may be computationally intensive task. However, in this research purpose, it was assumed as a known value. When the convective and diffusion processes of the local concentrations are known, the chemical or microbial conversion processes can be calculated with standard reaction kinetics, thus a new biomass is formed. The newly formed biomass in the previous step needs to be distributed for biofilm growth. Since there is no fundamental theory or good experimental observations for biomass spreading in biofilms the different models use different methods for this biomass spreading. Picioreanu et al. [8] and Hermanowicz [18] were used a discrete cellular automaton method for biomass spreading. In this method, surplus biomass is displaced to neighbouring cells, which lead to further displacement of the biomass in the neighbouring cells until an empty position at the biofilm-liquid interface is found. In several biofilm models, detachment equation is also included; however, equations are not based on any process [4]. The detachment term is only included in order to describe the occurrence of steady state of biofilm thickness. Picioreanu et al. [19] were the first to include a possible detachment mechanism based on the force exerted by the liquid flow. The mechanical stress in the biofilm is calculated and when it exceeds a certain level, the biofilm breaks leading to detachment.

2.2. Mathematical description

In this present model, a matrix representing nutrient concentrations is superimposed on the working space containing water and biomass [15]. However, only a single limiting substrate was considered, and in this case, oxygen. The model is developed by combining the rate expressions and mass balances. This is then used to predict the concentrations of substrate and biomass as a function of convective, diffusive and net production rate (growth rate). The growth rate that relates to bacterial cells is normally described using an expression known as the Monod model given by:

$$\mu_x = r_x = \frac{\mu_{\max} C_S}{K_M + C_S} \tag{1}$$

where μ_x is the specific growth rate depends only on the variable C_S. $\mu_{\max}$ is the maximum growth when the nutrient, C_S are present in sufficient amounts and K_M is the Monod constant describing the amount of substrate, C_S at the half of the maximum growth rate. Such a variation of μ_x with substrate, C_S makes it behaves in the same fashion as does the enzymatic rate described by the Michaelis–Menton kinetics. Besides Monod model, the rate of biomass formation and substrate consumption in the biofilm were also calculated in present study according to the kinetic model suggested by Beeftink and co-workers [11]. Other models were also based on the work by Picioreanu et al. [8,12]. The rate of substrate consumption in the biofilm that was considered in this study is given by a Monod function:

$$r_S = \frac{C_x}{Y_{x/S}} \frac{\mu_{\max} C_S}{K_M + C_S} = k \frac{\mu_{\max} C_S}{K_M + C_S} \tag{2}$$

In the model formulation, yield of biomass on oxygen,$Y_{x/S}$, and the biofilm biomass density, C_x, were lumped into one constant parameter, k, the consumption of oxygen.

The most basic principle for all quantitative models is conservation of mass. The net influx of mass is the difference between the mass brought into the system and the mass leaving the system [14]. Similarly, the net mass of a component generated in the system is the difference between production and consumption. At the microscopic level, mass balances can be written based on the above description. The mass balances are differential equations that express the variation of concentration of a component in time in a point in space as a result of transport and transformation processes. The mass balances are the mathematical form of equality, which in a Cartesian space, can be written as:

$$\frac{\partial C_i}{\partial t} = -\frac{\partial j_x}{\partial x} - \frac{\partial j_y}{\partial y} - \frac{\partial j_z}{\partial z} + r_x \tag{3}$$

where t is time; x, y and z are spatial coordinates; C_i is the concentration of component i; j_x, j_y and j_z are the components of the mass flux j along the coordinates; and r_x is the net production rate of the component [16]. Eq. (3) is the equation of continuity for a component, either soluble or particulate. Most commonly, the mass flux j is comprised of a diffusive flux j_D and a convective flux j_C. The diffusion flux in a direction, e.g., the z direction, is given by Fick's First Law:

$$j_{D,z} = -D \frac{\partial C_i}{\partial z} \tag{4}$$

where the diffusion coefficient,D, may be included. Besides the molecular diffusion, there is also turbulent diffusion that results from the movement of the fluid.

The convective flux is:

$$j_{C,z} = u_z C_i \tag{5}$$

where u_z denotes the z component of the carrying fluid velocity field. Substituting Eqs. (4) and (5) into Eq. (3) yields a second-order partial differential equation:

$$\frac{\partial C_i}{\partial t} = -\frac{\partial (u_x C_i)}{\partial x} - \frac{\partial (u_y C_i)}{\partial y} - \frac{\partial (u_z C_i)}{\partial z} + \frac{\partial}{\partial x}\left(D \frac{\partial C_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(D \frac{\partial C_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(D \frac{\partial C_i}{\partial z}\right) + r_x \tag{6}$$