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Analysis of the multidimensional effects in biofilms

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ABSTRACT

A general multidimensional, multispecies, heterogenous biofilm model is developed using the balance equations. Multidimensional effects are studied by taking limiting scenarios towards lower dimensional analogs, as well as studying the effects of changing biofilm surface geometries. Error maps are developed suggesting when single-dimensional models give an accurate representation of biofilm growth, and when multidimensional effects are substantial. A porous media model is studied, where the bacteria *Pseudomonas aeruginosa* is modeled to grow in a packed porous bed of spheres. It is found that under most circumstances, single-dimensional models predict very similar growth rates as compared to their multidimensional analogs. However, under some conditions the multidimensionality can have a significant effect in the model's predictions. To the authors' best knowledge, this is the first work which develops error maps detailing multidimensional effects of biofilm growth.

1. Introduction

Biofilms are communities of bacterial cells that are adherent to surfaces and are protected by a self-created extracellular polymeric substance. Free floating, planktonic bacteria can exhibit very different traits when compared to the same species of bacteria inhabiting a biofilm. In order for a biofilm to develop, a bacterial cell must adhere to a surface. From this point, other planktonic cells may attach to this initial cell, or instead they may also attach to the substratum. The attached bacteria then grow and divide, increasing the communal population of the biofilm. Through the use of quorum sensing, the bacteria can communicate their population and coordinate activation of various traits.

It is common for different species of bacteria to live together and compete for nutrients and space, thus multispecies and multisubstrate effects are important attributes to include in the development of comprehensive biofilm models. There exists a diverse set of methods used to model these interactions, with the most popular being to model the biofilm using continuum mechanics [1–5], individual-based models [6–8], cellular automaton [9,10], and combinations there-of [11,12].

Earlier work in biofilm modeling led to fairly simple yet powerful one dimensional continuum models, with one dimensional growth occurring orthogonal to the substratum [1,13,14]. One dimensional continuum models can have the ability to capture important effects, such as species competition for space and nutrients, which leads to a globally heterogenous biofilm structure [1]. Biofilm heterogeneity is a result of different species having different nutrient uptake rates, different growth rates and different EPS production rates. Heterogeneity in nutrient concentration is also captured in these one dimensional models, in part since different nutrients have different diffusion rates as well as different consumption rates. These are very important effects, which can be captured in one dimension.

Drawbacks to one dimensional models are that, for some cases which constitute a smaller subset of available scenarios, spatial heterogeneities do not necessarily occur only in the direction orthogonal to the substratum, but instead growth and diffusion processes can also occur parallel to that plane. If a spatial gradient exists in the nutrient concentration in the horizontal direction, then one would have a horizontal component of the nutrient flux. This would also result in bacterial species growing along this gradient, leading to a heterogeneous distribution of bacterial species in the horizontal direction within the biofilm. The impact of these types of growths needs to be assessed.

For example, in nutrient limited regimes and under conditions with sufficiently large mass transfer boundary layers biofilm fingering formation can occur [2,3], which is a multidimensional effect. This complex surface geometry affects nutrient diffusion processes, which itself affects species growth rates. By using one-dimensional models one is ignoring the effects of the surface geometry.

A second example of a multidimensional system is seen in a partially mixed multispecies system. One would expect to see spatial heterogeneities of bacterial species in the vertical as well as

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Nomenclature

Dependent variables

$\rho_s = \rho_s(x, y, z, t)$ density of species s
$v_s = v_s(x, y, z, t)$ volume fraction of species s
$C_n = C_n(x, y, z, t)$ concentration of nutrient n
$\vec{S} = \vec{u}(x, y, Z(x, y, t))$ parametric form of surface
$\vec{u} = \vec{u}(x, y, z, t)$ biofilm expansion velocity
$\Phi = \Phi(x, y, z, t)$ biofilm expansion potential

Reaction rates

$g_s = g_s(x, y, z, t)$ growth rate for species s
$r_n = r_n(x, y, z, t)$ reaction rate for nutrient n

Scaling factors

L_x domain width in x-direction
L_y domain width in y-direction
$Z = Z(x, y, t)$ functional form of surface
τ characteristic time scale

Constants

ρ_s^* density of species s
D_n constant scalar diffusion coefficient for nutrient n
λ biomass detachment coefficient
μ_s growth rate of species s
K_n^s monod saturation constant for species s and nutrient n
b_s endogenous rate constant for species s
k_s inactivation rate constant for species s
Y_s biomass yield for species s
α_s conversion factor for species s
$C_{n\mathrm{B}}$ bulk fluid concentration for nutrient n
i stoichiometric factor – EPS/*Pa*
k stoichiometric factor – Gl/O_2

Dimensionless variables

x' dimensionless x-variable
y' dimensionless y-variable
z' dimensionless z-variable
t' dimensionless time-variable

horizontal directions, and considering different bacterial species have different growth and consumption properties, these heterogeneities can lead to multidimensional species competition [2,6].

It is the purpose of this work to study and assess these multidimensional characteristics, their absolute influences on net growth rate, and finally to develop error maps which can be used to suggest when multidimensional characteristics are necessary for accurate prediction of biofilm growth.

2. Governing equations

The derivations of the governing equations have been influenced by previous work [1,2,4,5]. The biofilm is assumed to live in three spatial dimensions and one temporal dimension, i.e. $\mathbb{R}^3 \otimes \mathbb{R}$.

The biofilm is assumed to have continuous properties and growth will follow the continuity equation. Since biofilm expansion is convection dominated, for bacterial species s:

$$\frac{\partial \rho_s}{\partial t} + \vec{\nabla} \cdot (\vec{u}\, \rho_s) = g_s \tag{1}$$

The dependent variables are defined such that ρ_s is the density of species s, g_s is the growth rate of species s, and $\vec{u}$ is the biofilm expansion velocity. If it is assumed that the density of species s across the biofilm domain is constant $\rho_s^* \in \mathbb{R}$, then $\rho_s = \rho_s^* v_s$, where v_s is the volume fraction of species s in the biofilm. The biofilm growth equation becomes:

$$\frac{\partial v_s}{\partial t} + \vec{\nabla} \cdot (\vec{u}\, v_s) = \frac{g_s}{\rho_s^*} \tag{2}$$

Using the fact that $\sum_s v_s = 1$, one finds:

$$\vec{\nabla} \cdot \vec{u} = \sum_s \frac{g_s}{\rho_s^*}. \tag{3}$$

The growth equations can then be simplified to:

$$\frac{\partial v_s}{\partial t} + \vec{u} \cdot \vec{\nabla} v_s = \frac{g_s}{\rho_s^*} - v_s \sum_i \frac{g_i}{\rho_i^*} \tag{4}$$

Nutrient concentration for nutrient n within the biofilm is diffusion dominated and can be presented as:

$$\frac{\partial C_n}{\partial t} = D_n \nabla^2 C_n + r_n \tag{5}$$

The dependent variables are defined such that C_n is the nutrient concentration for nutrient n and r_n is the reaction rate. Since diffusion processes occur much faster than biofilm growth processes, and we are interested in biofilm growth processes, one may assume that the nutrient concentration has reached steady state over biofilm growth process time scales [15].

$$D_n \nabla^2 C_n + r_n = 0 \tag{6}$$

An order of magnitude argument can be made to justify this approximation. Diffusion coefficients of nutrients within biofilm are of order $D \sim 100 \times 10^{-6}$ m^2/days while lengths scales of biofilm are of order $l \sim 10^{-3}$ m, which imply that nutrient diffusion velocities within biofilm are of order $v_D \sim D/l \sim 10^{-1}$ m/days. Furthermore, biofilm grow to length scales of order $l \sim 10^{-3}$ m in $t \sim 10$ days, which implies that biofilm growth velocities are of order $v_G \sim l/t \sim 10^{-4}$ m/days. Thus diffusion velocities are 3 orders of magnitude greater than growth velocities, implying that the steady state approximation of nutrient diffusion is valid.

The parametric form of the biofilm surface $\vec{S}(x, y, t) = (x, y, Z(x, y, t))$ is related to the expansion velocity as follows:

$$\frac{\partial \vec{S}}{\partial t} = \vec{u}\,|_{z=Z} \tag{7}$$

The integral form of this differential equation is:

$$\vec{S} = \vec{S_o} + \int_0^t \vec{u}\, dt \tag{8}$$

One way in which shearing forces can be incorporated into the model is by modifying the differential equation for the biofilm surface [1]:

$$\frac{\partial \vec{S}}{\partial t} = \vec{u}\,|_{z=Z} - \lambda Z^2 \hat{z} \tag{9}$$

where λ is a constant specifying the relative strength of shearing forces.

The governing equations can be simplified by assuming irrotational growth [2,3]. The expansion velocity may then be taken as the negative gradient of a scalar potential $\vec{u} = -\vec{\nabla}\mathbf{\Phi}$. The governing equations in the final, coordinate-free form can be presented as:

$$\frac{\partial v_s}{\partial t} - \vec{\nabla}\mathbf{\Phi} \cdot \vec{\nabla} v_s = \frac{g_s}{\rho_s^*} - v_s \sum_i \frac{g_i}{\rho_i^*} \tag{10}$$