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2010

Papáček, Š. ; Matonoha, Ctirad. Effect of hydrodynamic mixing on the photosynthetic microorganism growth: Revisited.
In Seminar on Numerical Analysis. Modelling and Simulation of Challenging Engineering Problems.
Prague : Institute of Computer Science AS CR, 2010, S. 114-117. ISBN 978-80-87136-07-2.
[SNA '10. Seminar on Numerical Analysis, Nové Hrady, 18.01.2010-22.01.2010, CZ]

Effect of hydrodynamic mixing on the photosynthetic microorganism growth: Revisited

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1 Introduction

Biotechnology with microalgae and photo-bioreactor (PBR) design is nowadays regaining attention thanks to emerging projects of CO_2 sequestration and algae biofuels. Nevertheless, there do not exist reliable methods as well as programming software neither for modeling, simulation and control of microbial growth in photo-bioreactors, nor for PBR design [3]. Modeling in a predictive way the photosynthetic response in the three-dimensional flow field seems today unrealistic, because the global response depends on numerous interacting intracellular reactions, with various time-scales. The physiological state of any cellular system and its impact on growth and product formation is the result of a complex interplay between the extracellular environment and the cellular machinery. The design of PBR in which microalgae cells function as factories as well as the prediction of suitable PBR operating conditions is further complicated because of the dynamic variations of the extracellular environment.

Our main goal is to develop and implement the mathematical model of microalgae growth in a general PBR as tool in the design of photo-bioreactors and the optimization of their performance. In our previous works we studied an adequate multi-scale lumped parameter model which well describes the principal physiological mechanisms in microalgae: photosynthetic light-dark reactions and photoinhibition [5], as well as its model parameter estimation [8, 7]. In [6] we presented how to construct a distributed parameter model consisting mainly in determination of hydrodynamic dispersion coefficient as function of space coordinates.

This paper deals with the non-homogeneous steady-state one-dimensional reaction-diffusion system (3) with a special boundary condition. However, equation (3) is rewritten in form of two ordinary differential equations (ODE), which leads after re-scaling to the standard form of the singularly perturbed system [4]. The purpose of such an operation is to infer the asymptotic properties of the reaction-diffusion system (3).

2 Modelling photosynthetic microorganism growth

The photosynthetic microorganism growth description is usually based on the so-called microbial kinetics, i.e. on the lumped parameter models (LPM) describing the photosynthetic response in small cultivation systems with a homogeneous light distribution [9]. However, there is an important phenomenon, the so-called flashing light enhancement, which demands some other model than it residing in the artificial connection between the steady state kinetic model and the empiric one describing the photosynthetic productivity under fluctuating light condition. Nevertheless, even having an adequate dynamical LPM of microorganism growth, see e.g. phenomenological model of so-called photosynthetic factory [5, 8], another serious difficulty resides in the description of the microalgal growth in a PBR, i.e. in a distributed parameter system.

In order to develop the distributed parameter model (DPM) of a microorganism growth, two main approaches for transport and bioreaction processes modelling are usually chosen: (i) Eulerian infinitesimal, and (ii) Eulerian multicompartmental. While the Eulerian infinitesimal approach, leading to the partial differential equations (PDE), is an usual way to describe transport and reaction systems, the multicompartmental modelling framework, resulting in an ODE system, is mostly used in the process engineering area. This second approach, based on balance equation among compartments with finite control volume, has been recently treated by Bezzo *et al.* [2]. The authors presented there a rigorous mathematical framework for constructing *hybrid multicompartment/CFD models*. *Hybrid* there means that the fluid flow description is resolved by a CFD code, and does not make a part of the ODE system of governing equations.

In the sequel, we adopt the first approach aiming to clarify in an analytical manner the role of hydrodynamic mixing, or more precisely, the mechanism of the photosynthetic microorganism growth enhancement due to the microbial cell transport by radial dispersion. Nevertheless, in the future work, our results should serve to develop a numerical scheme for setting up the optimal compartment size in the multicompartment/CFD models.

3 Model development

Transport equation for microbial cells (concentration c) as the function of spatial coordinates and time gets the next form [1]:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{v}c) - \nabla \cdot (D_e \nabla c) = R(c) \ , \tag{1}$$

where $R(c)$ is the source term (representing microbial growth, unit: cell $\mathrm{m}^{-3}\mathrm{s}^{-1}$), $\mathbf{v}$ represents the velocity field, and D_e is the dispersion coefficient, which corresponds to diffusion coefficient in microstructure description and becomes mere empirical parameter suitably describing mixing in the system. D_e is influenced by the molecular diffusion and velocity profile. When mixing is mainly caused by the turbulent micro-eddies, the phenomenon is called the turbulent diffusion and a *turbulent diffusion coefficient* is introduced e.g. in [1]. The reaction obviously depends on some variables, usually called as substrates. For our special case of photosynthetic growth in a PBR, the role of only one limiting substrate (the nutrients are supposed to be present in a sufficient amount, i.e. they do not limit the growth) fulfills the irradiance, in other words, an external forcing input u. Moreover we suppose the rectangular PBR geometry illuminated from one side, i.e. the irradiance level is decreasing from the PBR wall to PBR core. Thus, the PBR volume (our computational domain) can be divided into layers with the same irradiance level, transforming the 3D problem into the one-dimensional. Consequently, the description of cell motion in direction of light gradient, i.e. perpendicular to PBR wall and at the same time perpendicular to the direction of convective flow, is of most interest. This motion is caused by the just mentioned turbulent diffusion. Furthermore, we can introduce the dimensionless spatial coordinate x, and the dimensionless dispersion coefficient $p(x)$ by

$$r := xL \ , \ D_e := p(x) \ D_0 \ ,$$

where L and D_0 (unit: $\mathrm{m}^2\mathrm{s}^{-1}$) are the PBR length in direction of light gradient, and a constant with some characteristic value, respectively.

Furthermore we introduce the dimensionless concentrations c and c_{ss} as

$$y := \frac{c}{c_m} \ , \ y_{ss} := \frac{c_{ss}}{c_m} \ ,$$

where c_m is a characteristic (e.g. maximal) concentration of c.

Based on the photosynthetic factory model [5, 8] we have for the reaction term R the relation

$$R(c) = -k\ (c - c_{ss})\ , \tag{2}$$

where k is the rate (unit: s^{-1}) associated with the dynamic process by which is the concentration c approaching to some value c_{ss} depending only on the external input $u(x)$.

As we are interested on the steady state solution of (1), i.e. $\frac{\partial c}{\partial t} = 0$, we finally obtain

$$-\left[p(x)y'\right]' + q(x)\ y = q(x)\ y_{ss},\ \ y'(0) = 0,\ y'(1) = 0\ , \tag{3}$$

where $q(x) := \frac{k(u(x))\ L^2}{D_0}$.

4 Asymptotic properties of the reaction-diffusion system (3)

In the process engineering literature, there exists a concept of well mixed unit. This construct is further used e.g. in the multicompartmental or multizonal models [2, 6]. The crucial question is: When a compartment with finite volume is well mixed? For a reaction-diffusion system, it has to depend on the so-called *Damköhler number*.

In our previous work, in sake of the benchmark problem, we were looking for an analytical solution of the equation (3). Realizing that it was impossible, we did not search the solution in the usual form of $y = y(x)$, but we wanted to find the mean value of y in the interval $x \in [0.1]$, i.e. to compute the expression $\int_0^1 y(x)\ \mathrm{d}x$. Based on [10], the boundary value problem (3) was transformed into the related initial value problem. It consisted in finding solutions of two homogeneous equations, two differential equations with the right-hand side and computing a solution of a system of two algebraic equations. By this procedure, we could have obtained a function value and its derivative in an arbitrary point. The original differential equation with boundary conditions was thus transformed into a differential equation with an initial condition. As we have needed only a solution in several points, we could apply the above procedure repeatedly. Finally, the value $\int_0^1 y(x)\ \mathrm{d}x$ would be obtained by a suitable numerical method.

Now, we are developing an asymptotic method. Let first define $\frac{\mathrm{d}}{\mathrm{d}x}y := z$, then the resulting first order ODE system is

$$\frac{\mathrm{d}}{\mathrm{d}x}y = z\ ,\ \frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)z\right] = q(x)\ (y - y_{ss})\ ,\ z(0) = 0,\ z(1) = 0\ \ . \tag{4}$$

Consequently, if we define k_0 as follows: $k := k_A(u(x))\ k_0$, then the *Damköhler number* of second type could be defined as $Da_{II} := \frac{k_0 L^2}{D_0}$, and the dependence of the solution of (4) on $Da_{II} := \varepsilon \to 0$ could be studied.

The following ODE (5)

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)z\right] = \varepsilon k_A(u(x))\ (y - y_{ss})\ ,\ z(0) = 0,\ z(1) = 0\ \ , \tag{5}$$

thanks to the properties of its right hand side clearly satisfies the sufficient condition for applying the averaging method [4]. One can therefore approximate (4) as follows (always when $\varepsilon \to 0$):

$$\frac{\mathrm{d}}{\mathrm{d}x}y = z\ ,\ \frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)z\right] = \varepsilon \int_0^1 \left[k_A(u(x))\ (y - y_{ss})\right] \mathrm{d}x\ ,\ z(0) = 0,\ z(1) = 0\ \ . \tag{6}$$

Acknowledgement: This work was supported by the grant MŠMT MSM 600 766 58 08 of the Ministry of Education, Youth and Sports of the Czech Republic, and by the Grant Agency of Czech Republic through the research grant No. 102/05/0011.

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