MODELLING AND SIMULATION OF PHOTOSYNTHETIC MICROORGANISM GROWTH: FINITE DIFFERENCE METHOD VS. RANDOM WALK

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1 INTRODUCTION

An adequate model of microalgae growth is of paramount importance both for the optimal photobioreactor (PBR) design and the optimal PBR control (i.e. to optimize operating conditions, see e.g., Papáček et al., 2008). Nevertheless, even having an adequate dynamic lumped parameter model (LPM) of microalgae growth, another serious difficulty resides in the description of microorganism growth in a PBR, i.e. in a distributed parameter system. Because the traditional scale-up methodology of PBR design fails, in the next section we explain how to 'extend' the LPM into 3D.

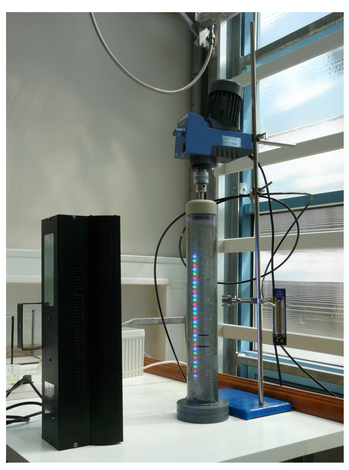


Fig.1: Couette-Taylor PBR, AUC, N.Hrady, see Papáček et al. (2007b).

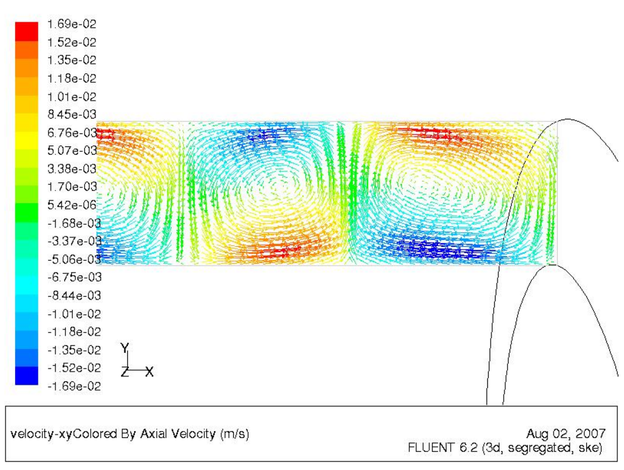


Fig.2: Flow field in axial section of Couette-Taylor PBR computed by CFD code Fluent, Papáček et al. (2007b).

2 MODEL DEVELOPMENT

2.1 Governing equations of algal growth – LPM

The photosynthetic microorganisms growth is usually modeled as the steady-state light response curve (so-called *P–I curve*), which represents the microbial kinetics (either of *Monod* or *Haldane* type). However, in order to describe some dynamic phenomena, e.g. the flashing light enhancement (Davis, 1953), a dynamic model is needed. The problem is even more complicated due to the fact that the relevant transport and reaction phenomena operate in very different time-scales, for more detail see Papáček et al., 2007b. Nonetheless, the phenomenological three-state model of photosynthetic factory (PSF model) proposed by Eilers & Peeters (1993) and further developed by Papáček et al. (2007a), correctly describes the principal physiological mechanisms: photosynthetic light-dark reactions and photoinhibition, see Fig.3 below. For the PSF model parameter $(\alpha, \beta, \gamma, \delta)$ estimation, see Rehák et al. (2008).

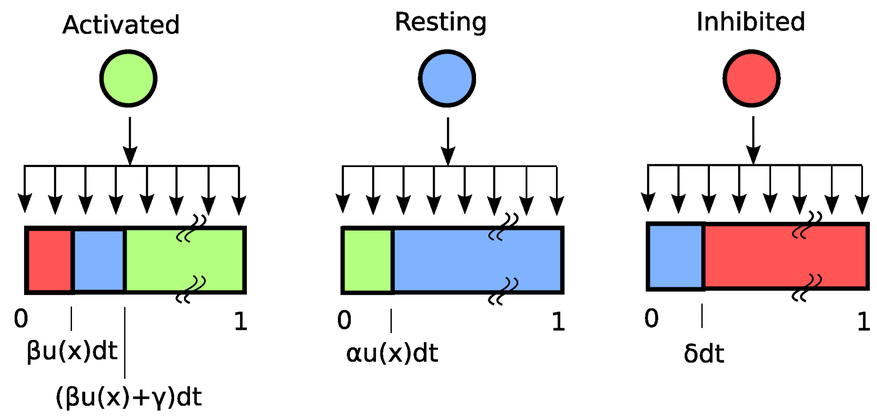


Fig.3: Three-state model of photosynthetic factory (PSF model) proposed by Eilers & Peeters (1993), terms below the rectangles indicate the probability of respective transitions.

2.2 DPM of algal growth – Eulerian approach

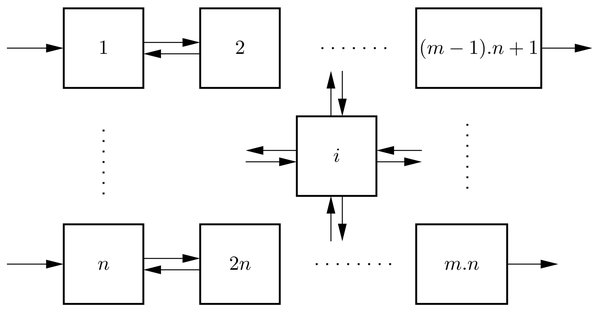
The systems with distributed parameters are usually described by means of partial differential equations (PDE). The PBR as Convection-Reaction-Diffusion (Dispersion) System is thus represented by the folowing governing equations:

$$\frac{\partial c_A}{\partial t} + \nabla \cdot (\vec{v} c_A) - \nabla \cdot (D \nabla c_A) = -k(c_A - c_{Ass}) \ , \qquad (1)$$

where c_A is cell-in-state-A(activated)-concentration (unit: cell m^{-3}), $\vec{v}$ represents the velocity field, D is the hydrodynamic dispersion coefficient and k (unit: s^{-1}) is the rate at which the concentration c_A is approaching to its steady-state value c_{Ass}. Similar equation could be written for the cell-in-state-R(resting)-concentration and for the cell-in-state-B(inhibited)-concentration, unless the method of order reduction is used, see Papáček et al., 2008. Usually k depends on some external input (forcing) u, e.g. $k(u) = \theta_1(u(x) + \theta_2)$, where according to Lambert-Beer law: $u(x) = u_0 \exp(-\tau x)$. The above PDE (1) has to be solved simultaneously with the Navier-Stokes equation system, e.g. by a Finite Difference Method (FDM) or by a commercial CFD code, e.g. Fluent, see Fig.2.

2.3 Multicompartment/CFD approach - ODE based DPM of algal growth

A fresh approach, leading to the model of 'well mixed' interconnected vessels (compartments) with lumped parameters, see Fig.4, and ODE system (2), was studied in Bezzo et al. (2003). Usually the fluid dynamics operates on a much faster time-scale than the reaction, therefore it is not necessary to calculate the reaction term in each time step and every point as the CFD code does for the fluid flow. Moreover, the compartment volumes can be of several orders bigger than that for CFD simulation.



$$V_i \frac{\mathrm{d}c_i}{\mathrm{d}t} = \left[\sum_{j=1}^{n_i} (c_j \ f_{ji} - c_i \ f_{ij}) S_{ij} \right] + V_i \ R_{c_i} \qquad (2)$$

While the problem of reaction term (matrix) R_{c_i}, and mass transfer coefficients f_{ij} determination was treated in Papáček et al. (2007b), the problem *How to set-up the optimal compartment size? I.e. how to reconcile the discretisation based on the hydrodynamic conditions with the discretisation based on the irradiance profile?* is still waiting for a convincing solution.

2.4 DPM of algal growth – Lagrangian approach

The Lagrangian treatment of the motion of each individual algal cell has the advantage that many effects observed in small systems, e.g. flashing light enhancement and the shear stress influence on growth (counting with the 'cell memory'), can be directly incorporated into our model. That is, having an accurate LPM of microalgal growth, it can be relatively simply applied to a system with spatially distributed parameters via Lagrangian formulation. The problem formulation is now 'stochastic', i.e. the trajectories simulation is performed using random walk techniques, see Papáček et al. (2007b), and the transitions among states are governed by the conditional probabilities depicted in Fig.3.

3 CONCLUSION

We presented some approaches for photosynthetic microorganisms growth modelling and simulation. The 'classical' approach is based on PDE (reaction-hydrodynamic dispersion system) and CFD. Some innovation is put into Multicompartment/CFD approach. Lagrangian approach naturally allows us to involve the 'cell memory' into the growth model. For all three approaches, the complications residing in modelling of multi-scale transport and reaction phenomena were clarified. An innovative solution consisting on the phenomenological state description of microalgal culture (PSF model) rather than on real microalgal cell concentration, has been chosen. Our future goal is to evaluate the advantages and inconveniences of each approach performing the simulation of some benchmark case study.

Acknowledgement

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