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A RANDOM WALK MODEL OF DISPERSION IN PHOTOBIOREACTORS AND ITS APPLICATION TO MODELLING OF MICROALGAL GROWTH

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Summary: *A problem of microalgal growth modeling is presented. The hybrid multicompartment/CFD approach, introduced by Bezzo et al. (2003), is deeply analyzed and recommended for the processes with much faster fluid dynamics time-scale than the reaction rate. The method resides in photobioreactor division into a network of well-mixed compartments and in description of mass transfer among adjacent compartments. Photosynthetic reactions and other related phenomena are described in each compartment by an ordinary differential equation. The flow of microalgal culture in suspension is calculated by the steady-state computational fluid dynamics (CFD). Then the single cell trajectories are simulated using the random walk model of dispersion. The relative flow rates are derived from several thousand predicted trajectories according to our original methodology.*

1. Introduction: Algal biotechnology basics

Algal biotechnology and photobioreactor (PBR) design is a promising field in the bioreaction technology and engineering; see Figures 1-3 for three different geometries of PBR, designed and operated either at the Academic and University Centre, Nove Hrady, Czech Republic or at the Institute of Microbiology of the Academy of Sciences of the Czech Republic. The main difference between the cultivation of chemoheterotrophs (fungi, bacteria, etc.) and phototrophs (microalgae and cyanobacteria) is that, in the latter case, the energy source can not be stored in the culture medium, but it must be continuously provided. Delivering the light in an optimal manner, achieving maximum productivity is a key issue in photobioreactor design and operation. When microalgal cells are grown in a PBR, the irradiation decreases exponentially with distance from an irradiated PBR side, according to the Beer-Lambert law. The cells near the front are exposed to a higher irradiation allowing a high growth rate. At the core, the cells receive less light and will thus have a lower growth rate (Masojídek et al.,

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2003). The crucial role in whole story plays the hydrodynamic mixing in direction of irradiance gradient (i.e. the radial dispersion for the case of cylindrical geometry). Due to the hydrodynamic mixing, the microbial cells are moving between the front and core of the PBR and receive the light intermittently. The light-dark cycling of an appropriate frequency and average irradiance could enhance the specific growth rate, and is known as the flashing-light effect. The mechanism of productivity enhancement is studied since 1950, however, remains unknown.

Fig. 1: Tubular photobioreactor with linear Fresnel lenses, AUC, N. Hrady.

Fig. 2: Couette-Taylor PBR, AUC, N. Hrady.

Fig. 3: Flat panel PBR, MBU, Třeboň.

Nevertheless, the mechanistic three-state model of photosynthetic factory – PSF model, proposed by Eilers & Peeters (1993) and further developed by Papáček et al. (2007), Rehák et al. (2008), fulfils two basics requirements for the microalgae growth model: (i) the steady-state microbial growth kinetics is of *Haldane* type, and (ii) the model has so-called light integration property, i.e. as the light-dark cycle frequency is going to infinity, the value of resulting production rate (e.g. photosynthetic oxygen evolution rate) goes to a certain limit value, which depends on average irradiance only. Consequently, the PSF model is taken in the sequel as our lumped parameter model (LPM) of microalgal growth.

2. Distributed parameter model (DPM) development

Having an adequate model of microalgal growth in PBR is of paramount importance for the optimal design of a PBR and for the optimization of PBR operating conditions. The models describing microalgal growth in a distributed parameter system were usually based on the empirical description of microbial kinetics in small cultivation systems with a homogeneous light distribution; i.e. on the steady-state characteristic, so-called *P–I curve*. Thereafter, the interconnection between the steady-state model and the dynamic one was often artificial. Nevertheless, even having an adequate dynamical LPM of microalgal growth (see e.g. phenomenological PSF model) another serious difficulty resides in the description of the microalgal growth in a photobioreactor, i.e. in a distributed parameter system. The traditional scale-up methodology of PBR design does not work, that is the reason why a novel method was recently proposed (Papáček et al., 2007b), and in this paper is further developed. The scheme of three main phenomena to model is presented in Figure 4. While the topic of irradiance distribution and biochemical reaction was partly treated in the Introduction, the mass transfer phenomena will be studied in the subsequent sections. Now, let us remark that the mixing properties are entirely defined by the dispersion coefficient. To calculate it, the information on velocity and turbulent mixing (that is often not known) is required. It is therefore more common to estimate the coefficient from empirical equations or to use tracer experiments. In the modelling process (before having a real device), we have to look for another method. Random walk model is an alternative: A large number of particles (algal cells) are tracked as they move through a numerical representation of the flow field (effectuated by a CFD code). The particles follow the local time averaged velocity for each time step of the simulation and are given a random motion to model the turbulent mixing. Only after having the trajectories, the cell growth could be modelled (e.g. in a special laboratory PBR where the condition of light use and the condition of hydrodynamic stress are uniform; which is the case of Couette-Taylor PBR, Fig. 2). Finally, we resume: (i) the study of all three phenomena in Fig. 4 should not be completely decoupled, and (ii) the crucial role in the fluid dynamics modelling plays the trajectory simulation of each individual microalgal cell.

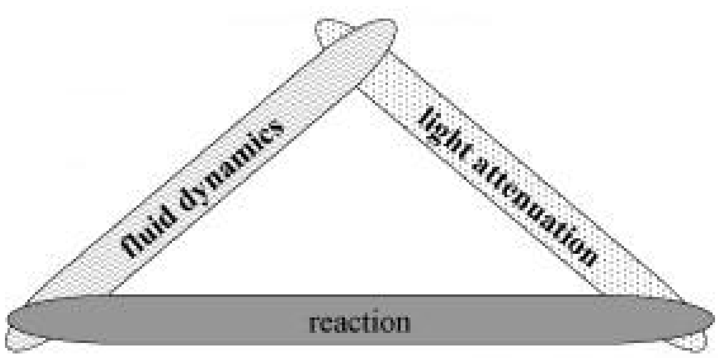

Fig. 4: The schematic presentation of three basic phenomena interconnection (light attenuation, fluid dynamics and biochemical reactions) during the cultivation of microalgae in photobioreactors.

2.1. Lagrangian approach

There are two main approaches for transport and reaction processes modelling in algal biotechnology: (i) Lagrangian and (ii) Eulerian. 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, can be directly incorporated into PBR model. That is, having an accurate LPM of microalgal growth, it can be directly applied to a system with spatially distributed parameters via Lagrangian formulation. For a known irradiance distribution in PBR, the irradiance history for each microalgal cell could be received by coupling the microalgal cell trajectories with the scalar field of irradiance. This time course of irradiance of an individual microalgal cell represents the stochastic input variable $u(t)$ for LPM. For the three-state model PSF model (x is state vector, A and B are matrices of rate constants of appropriate dimensions), the governing equation has the following form:

$$\dot{x} = Ax + Bx\,u(t)\ . \quad (1)$$

Behind this apparently simple ordinary differential equation system reside the troublesome identification of the input variable for different PBR design parameters and operating regimes. This is why we look for a better modeling framework.

2.2. Eulerian infinitesimal approach

The ordinary description of systems with distributed parameters is by means of partial differential equations (PDE). In our case, when the reaction rate is modeled by the PSF model (1), the only problem is how to describe the mass transfer in direction of light gradient, i.e. perpendicular to PBR wall and at the same time perpendicular to the direction of convective flow, i.e. how to determine the dispersion coefficient. An evident inconvenient of this approach is that the fluid dynamics operates on a much faster time-scale than the reaction and it is unnecessary expensive to calculate the reaction term in each time step and every point as the CFD code does for the fluid flow. Hence, in the paper Bezzo et al. (2003) was introduced a new idea how to model this type of transport and reaction processes; see the following subsection.

2.3. Multicompartment approach

The decision to study the macroscopic properties in the macroscopic control volumes instead of microscopic (infinitesimal) ones leads to the model of interconnected vessels or compartments with lumped parameters. The resulting mathematical description consists of the system of ordinary differential equations; see Papáček et al. (2007b) for more details. An apparent problem arises when we look for PBR spatial discretisation: How to reconcile the discretisation based on the hydrodynamic conditions (”well mixed compartment” should be well mixed!) with the discretisation based on the irradiance profile? Unexpectedly, the problem has an elegant solution: Apart from the material quantities, also the light could be ”mixed” inside the well mixed compartment if the adequate model for photosynthetic reaction is chosen. This fact harmoniously links the different disciplines involved in PBR modeling (i.e. hydrodynamics, optics and microbiology, see Fig. 4) and leads to the conclusion that likewise the material substances, also irradiance can be averaged inside the compartment volume always when the mean residence time in each compartment is in the same time-scale as the reaction. How to determine the mass flow rate between adjacent compartments? This is the topic of the following section.

3. Mass transfer between adjacent compartments

3.1. CFD simulations of single algal cell trajectories: Random walk model

CFD simulation of particle trajectories was performed by CFD code Fluent. The dispersion of particles was modeled using a stochastic discrete-particle approach, so-called Discrete Random Walk – DRW model. For the case of Couette-Taylor photobioreactor – CTBR (Fig. 2), a single algal cell trajectory is shown in Fig. 5:

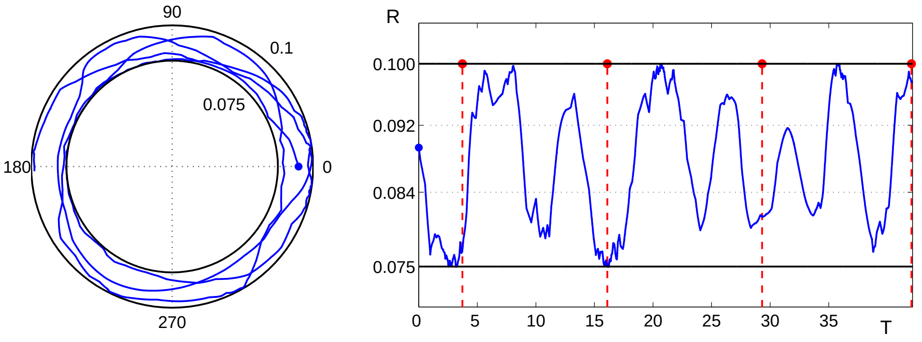

Fig. 5: The single algal cell (particle) trajectory inside Couette-Taylor photobioreactor: (i) Top-view – on the left, and (ii) Time-course of the radial position – on the right.

3.2. Post-processing of particle trajectories

For the above mentioned case of Couette-Taylor photobioreactor, the 7552 particles were released from a plane containing CTBR axis. The flow rate between adjacent compartments was based on the counting of particles crossing the inter-compartment border. The coordinates of each of 7552 particles were post-processed using MATLAB, and the dependency of the number of particles crossing a coaxial surface S_{ij} on time was drawn (see Fig. 6). The values of the inter-compartment flow rates f_{ij} are derived according the following relation

$$f_{ij} := \lim_{t \to \infty} \frac{1}{t} \frac{N_{ij}^{+}}{N_T} \frac{V}{S_{ij}} \tag{2}$$

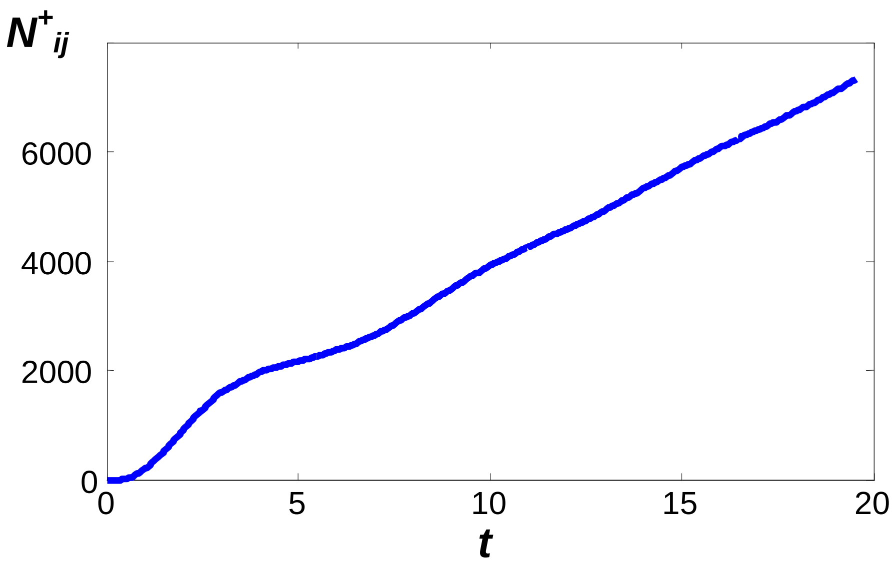

Fig. 6: Time course of the number of particles crossing the ***i-j*** inter-compartment border.

4. Conclusions

The main purpose of this paper was to describe how to model the hydrodynamic mixing in a photobioreactor (i.e. the *turbulent diffusivity* or the *hydrodynamic dispersion*) in order to determine the growth of microalgae in suspension. It was presented the motivation of this effort, i.e. the promising multicompartment modelling framework which optimally (i.e. finding the trade-off between precision and computation cost) describes the transport and photosynthetic reaction processes in a general PBR. The reason for using this hybrid multicompartment/CFD approach was explained: Firstly, while the Lagrangian formulation makes troublesome the identification of input variable for the process model, the simple modular principle of spatial discretisation of PBR volume is the main advantage of the compartmental approach. Secondly, the other advantage of the multicompartment/CFD approach is the fact that the compartment size can reflect the peculiarity of biochemical processes, i.e. the compartment volumes can be of several orders bigger than that for fluid flow calculation by some CFD software. Moreover, the recent methodology for inter-compartment flow rates estimation, based on the CFD simulations of single algal cell trajectories (*via* Discrete Random Walk model) and the subsequent counting of number of particles crossing the border between adjacent compartments, reveals very good qualitative properties (see Fig. 6).

Our future goals are related to the application of the presented modeling framework, in order to compare the behaviour of CTBR model with a real device (i.e. performing a growth experiment in our laboratory CTBR).

Acknowledgement

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