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Multicompartment/CFD modelling of transport and reaction processes in Couette-Taylor photobioreactor

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Abstract

A hybrid multicompartment/CFD modelling approach, introduced by Bezzo *et al.* (2003), describing processes with much faster fluid dynamics time-scale than the reaction rate, is used to characterise microalgal growth in a photobioreactor. Our system of interest, the Couette-Taylor bioreactor (CTBR), is divided into a network of well-mixed compartments. Photosynthetic reactions and other related phenomena are described in each compartment by an ordinary differential equation (ODE). The flow of neutrally-buoyant particles, representing a continuous mass flow of microalgal cells inside CTBR, is simulated by a steady-state computational fluid dynamics (CFD) computations. The flow rates between adjacent compartments are derived from several thousand predicted trajectories, post-processed using MATLAB®, accordingly to our original method. The resulting governing equations are formed as a system of n_c (total number of compartments) ODE's, which are easier to handle than the large system of equations rising from a reaction phenomena incorporated in CFD models.

Keywords: CFD, multicompartment modelling, photobioreactor, microalgae

1. Introduction

The models describing microalgal growth are usually based on the empirical description of microbial kinetics in small cultivation systems with a homogeneous light distribution (i.e. on the so-called P–I curve [9, 13, 23, 25]). Thereafter, the interconnection between the steady state kinetic model and the dynamic one is often artificial (see e.g. the well-known flashing light experiments [17, 27]). Nevertheless, even having an adequate dynamical lumped parameter model (LPM) of microalgal growth (see e.g. phenomenological model of so-called photosynthetic factory [10, 11, 29, 19, 20]), another serious difficulty resides in the description of the microalgal growth in a photobioreactor (PBR), i.e. in a distributed parameter system. Both main approaches for transport and reaction processes modelling were employed in algal biotechnology: (i) Lagrangian in [21, 22, 30]), and (ii) Eulerian in [18, 19]. This topic will be further discussed in the following subsections.

1.1. 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 [14], can be directly incorporated into PBR model. That is, having an accurate LPM of microalgal growth, it can be

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directly applied to a system with spatially distributed parameters via Lagrangian formulation, see e.g. [30]. 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 [8, 19]. This time course of irradiance of an individual microalgal cell represents the stochastic input variable for LPM.

1.2. Eulerian infinitesimal approach

The systems with distributed parameters are mainly modelled by means of partial differential equations (PDE). Accordingly to [28], the transport equation for microalgal cells (concentration or cell density c) as the function of spatial coordinates and time gets the next form:

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

where R is the reaction (growth) rate (unit: cell $\mathrm{m}^{-3}\mathrm{s}^{-1}$), $\vec{v}$ represents the velocity field, and D_e is the dispersion coefficient.[1] For our special case of photosynthetic growth, we suppose the uniform cell density in the layers with uniform irradiance level, thus the description of microalgal 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 and the transport equation in *transversal* or *radial* (in case of cylindrical geometry) direction can be described in dimensionless form (indicated by an over-line) as follows:

$$\frac{\partial \overline{c}}{\partial \overline{t}} = \overline{\nabla} \cdot \left[\frac{D_e(r,c)}{{D_e}^*} \overline{\nabla} \overline{c} \right] + \mu(r) \frac{d^2}{{D_e}^*} \,, \tag{2}$$

where $\bar{t}$ is the dimensionless time ($t = \bar{t} \frac{d^2}{{D_e}^*}$), $\mu(r)$ is the specific growth rate of microalgal growth (representing reaction kinetics, unit: s^{-1}), which depend on irradiance level depending on a spatial coordinate, e.g. $I(r) = I_0 \, e^{-k_a r}$ (Lambert-Beer law), d represents the characteristic length in transversal direction, and ${D_e}^*$ is the characteristic dispersion coefficient. The term $\mu \frac{d^2}{D_e}$, which submits into relation the characteristic time of dispersion and this of algal growth, is called the second *Damköhler number* – $\mathrm{Da}^{\mathrm{II}}$. Equation (2) can be solved by means of numerical methods, e.g. FDM, FEM, FVM. However, we can expect some numerical difficulties while solving Eq. (2), because $\mathrm{Da}^{\mathrm{II}}$ reaches the values in order of 10^{-3} in our specific case, which could be also interpreted as the loss of sensitivity to the reaction term. In other words, fluid dynamics operates on a much faster time-scale than the reaction. The difficulties should disappear for an other process model being sensitive to the characteristic time of cell transport in direction of light gradient. A more adequate model of photosynthesis will be introduced only in the section 2: Model development.

1.3. Multicompartment approach

The Eulerian approach based on finite control volume and mass balance equation has been introduced by Bezzo *et al.* [5, 6]. The authors presented there a rigorous mathematical framework for constructing hybrid multicompartment/CFD models. Their work generalizes and unifies much of the work on hybrid multicompartment/CFD models presented in earlier literature

[1] The dispersion coefficient D_e 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 microeddies, the phenomenon is called the turbulent diffusion and a *turbulent diffusion coefficient* is introduced e.g. in [4].

[1, 2, 3, 24]. However, a problem common to all these hybrid models is the cost associated with the CFD calculations. More specifically, the CFD submodel is essentially embedded within a multicompartment process model and the submodel output quantities y (such as an intercompartment flow rate or the volume-averaged turbulent energy dissipation rate) for the given set of inputs x (such as the density and viscosity of the fluid in each compartment) may need to be evaluated hundreds of times during a typical steady-state or dynamic simulation. Even with some form of hot-start of the CFD calculations after the first evaluation, the resulting computational cost may still be prohibitive.

The last paper of Bezzo *et al.* [7] examines ways of addressing the above problem. The basic idea is that a relatively large proportion of the evaluations of the function $y = F(x)$ are replaced by evaluations of local approximate models of the form $y = f(x, \alpha)$ where the values of the parameters α are estimated by fitting the results of evaluations of the original function $F(\cdot)$ carried out earlier during the solution of the hybrid multicompartment/CFD model.

In our specific case of CTBR when the small number of inputs are involved, the so-called response-surface technique looks as very promising method (for more detail see e.g. [12]), and this work is its first application in PBR modelling.

Our paper is organised as follows. The next section describes the PBR model development, introduces the PSF model and defines some relevant quantities. Section 3 presents the novel method for identifying the flow rates between adjacent compartment from CFD simulations. Final section draws some conclusions and gives some outlooks for future work.

2. Model development

2.1. Governing equations of algal growth in CTBR

The decision to study the macroscopic properties in the *macroscopic control volumes* instead of microscopic 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 (ODE), see Eq. (3):

$$V_i \frac{\mathrm{d}c_i}{\mathrm{dt}} = \left[\sum_{j=1}^{n_i} (c_j \, f_{ji} - c_i \, f_{ij}) S_{ij} \right] + V_i \, R_{c_i} \quad , \quad i \in 1, 2, ..., n_c \quad , \tag{3}$$

where c_i is the cell density in $i - \mathrm{th}$ compartment, V_i is the volume of $i - \mathrm{th}$ compartment, S_{ij} is the common surface between $i - \mathrm{th}$ and $j - \mathrm{th}$ compartment, the coefficients f_{ij} represent the flow rates per unit area (unit: m s^{-1}) from $i - \mathrm{th}$ compartment to $j - \mathrm{th}$ compartment, the total number of neighbour compartments to the $i - \mathrm{th}$ compartment is n_i, n_c is the total number of all compartments, and R_{c_i} is the reaction rate corresponding to $i - \mathrm{th}$ compartment. This approach is conditioned by the *ideal* or *well mixing*, which means that in the whole compartment the same material composition is kept [28].

When c_i represents the "local" algal cell density, then in the time-scale of cell transport (either by convection and dispersion) c_i reaches the nearby identical values in whole PBR (the growth rate is in order of 10^{-5} s^{-1} in our specific case of a microalgal culture). Consequently from (3) the transport term can be cancelled by extracting $c_i \cong c_j$ from the sum, and subsequently applying the continuity equation, i.e. $\sum_{j=1}^{n_i} (f_{ji} - f_{ij}) = 0$. This fact can be interpreted as the loss of sensitivity to the transport term. However, it would be contradictory to the experimental results based on the so-called "flashing-light experiments" [17]. We present its solution in the next subsection.

An other problem arises when we look for PBR spatial discretisation: How to reconcile the discretisation based on the hydrodynamic conditions (the "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 created.[2] This fact harmoniously links the different disciplines involved in PBR modelling (i.e. hydrodynamics, optics and microbiology) 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. Hence, although the classical treatment of the transport and reaction processes (TRP) consists of the problem division and separate study of each part, we took advantage of the common study of TRP in PBR. Fortunately in the next, after a common analysis of our problem, the fluid flow can be solved separately from the process dynamics. This fact represents the main advantage of the compartmental approach over the Lagrangian, i.e. one big problem (reaction and transport) can be divided into two simpler ones.

2.2. Determination of reaction rate R_{c_i} based on PSF model

Viewing the insurmountable difficulties in modelling cell growth directly (this difficulties reside in fact that the relevant phenomena operate in very different time-scales, for more detail see Subsection 1.2. and [19]), we opt for a phenomenological model which covers the principal physiological mechanisms. We suppose that the microalgal cells exist (with certain probability) in one of three hypothetical states (*activated, inhibited* and *rested*) of the so-called model of photosynthetic factory (PSF). Though the fluid-dynamical properties of cells in each of three states are identical, the description of the temporal and spatial dependence of molar concentrations of cells in respective states (similarly to the description of concentration of three different components of one phase), is very useful for further evaluation of microalgal growth (see Eq. 5). Let be the concentrations of respective components c_A, c_B, and c_R (with the same units as for the cell density c in whole PBR – generaly 10^6 cell ml^{-1} as in [29]). Then the following relation holds (for $\forall t \in [t_0, t_\infty]$, and for all point in PBR):

$$c_{Ai} + c_{Bi} + c_{Ri} = c_i \ , \tag{4}$$

where i represents index of a control volume (spatial index). Due to sufficient mixing holds: $c_i \approx c$, then dimensionless scalar values $x_R = c_R/c$, $x_A = c_A/c$, and $x_B = c_B/c$ (molar fractions) are respective states of the PSF model. According to [10], the rate of photosynthetic production (or the specific growth rate $\mu := \dot{c}/c$) is:

$$\dot{c} = \kappa\gamma \, x_A \, c = \kappa\gamma \, c_A \ . \tag{5}$$

This equation point out the necessity to determine the time course of x_A or c_A in each compartment, in order to describe the cell growth in whole PBR.[3] The states of PSF model are described

[2] It is proven in [19] and more rigorously in [20], that for the PSF model the resulting microbial growth in certain volume of the algal culture is approaching (while the extent of mixing is growing) the limiting value, which only depends on average value of the relevant variables in the volume. This theoretical result is in concord with the experimental data published e.g. in [27, 17].

[3] It is worth to note that the term $\kappa\gamma$ in (5) is of the order 10^{-5} [s^{-1}], while the state x_A of the PSF model is in range of 0 and 1 [-] and it is sensitive to the light fluctuation either due to fluid dynamics and the light source. By this way, the transition from the time-scale of light fluctuation (time micro-scale) to time-scale of biomass growth (time macro-scale) is effectuated without loss of accuracy.

by the system of three ODE:

$$\begin{bmatrix} \dot{x}_R \\ \dot{x}_A \\ \dot{x}_B \end{bmatrix} = \begin{bmatrix} 0 & \gamma & \delta \\ 0 & -\gamma & 0 \\ 0 & 0 & -\delta \end{bmatrix} \begin{bmatrix} x_R \\ x_A \\ x_B \end{bmatrix} + u(t) \begin{bmatrix} -\alpha & 0 & 0 \\ \alpha & -\beta & 0 \\ 0 & \beta & 0 \end{bmatrix} \begin{bmatrix} x_R \\ x_A \\ x_B \end{bmatrix}, \tag{6}$$

where $\alpha, \beta, \gamma, \delta, \kappa$ are rate constants of PSF model (δ is the rate of recovery from the inhibited state) and $u(t)$ is the known scalar input function. It is assumed that $u(t)$ is at least piecewise continuous. The ODE system (6) is *stiff* and the stiffness ratio is about 10^3 (slightly depending on u), for more detail see [10, 11, 19, 20]. The eigenvalues λ_1 and λ_2 (units: s^{-1}) are negative for every $u \geq 0$, and correspond to the processes with fast (photosynthetic light/dark reactions) and slow dynamics (photoinhibition).[4]

The ODE system (6) can be immediately reduced using the identity: $x_R + x_A + x_B = 1$, derived from (4). Moreover, having in mind that the slow state x_B for slowly changing $u(t)$ is nearby constant, we receive only one ODE in this case (i.e. $\dot{u}(t) \approx 0$):

$$\dot{x_A} = -\left[(\alpha + \beta)u(t) + \gamma\right] x_A + \alpha u(t) \left[1 - x_{Bss}(u_{av})\right] \ . \tag{7}$$

Eq. (7) describes the fast dynamics of activated state x_A, while the inhibited state x_B reaches its steady state: $x_{Bss}(u_{av}) = \frac{\alpha\beta u_{av}^2}{\lambda_1 \lambda_2}$ depending on the averaged value u_{av}). The governing equation for the concentration of component c_A is then:

$$V_i \frac{\mathrm{d}c_{Ai}}{\mathrm{dt}} = \left[\sum_{j=1}^{n_i} (c_{Aj}\ f_{ji} - c_{Ai}\ f_{ij}) S_{ij}\right] - \left[(\alpha + \beta)u_{iav} + \gamma\right] x_A + \alpha u_{iav} \left[1 - x_{Bss}(u_{av})\right]\ V_i\ c, \tag{8}$$

$$i \in 1, 2, ..., n_c \quad ,$$

where the reaction term was determined by (7), where $u(t) = u_{iav}$, which is the average irradiance in compartment i (while u_{av} is the average irradiance in whole PBR). The irradiance distribution in a PBR can be determined theoretically (this is mainly the case in the PBR design process) or experimentally. The governing equation (8) can be readily solved (having estimated the set of model parameters and the initial conditions). Consequently, integrating over time and space we receive the relation between the specific growth rate in whole PBR and the model inputs. In the next section, the transport of microalgal cells inside Coutte-Taylor photobioreactor in order to estimate the flow rates between adjacent compartments will be studied.

3. CTBR fluid dynamics and CFD simulations

The main reason to study the PBR fluid dynamics is to determine flow rates between adjacent compartments. These can be calculated by means of steady-state CFD calculations. Also the other fluid mechanical quantities that have important effects on the growth of microalgal cells (such as the shear stress on the filamentous cyanobacteria *Spirulina*) can be determined within each compartment. Nevertheless, in this paper we suppose that the biochemical reaction (algal growth) is depending on light availability within each compartment only, thus it is only the inter-compartmental flow rate which is in scope of interest.

[4] The eigenvalues were calculated for the irradiance u = 250 $\mu\mathrm{Em}^{-2}\mathrm{s}^{-1}$ resulting in λ_1=-0.63, λ_2=-0.59 10^{-3}, when the following PSF model parameters were taken from [29] (for the microalga *Porphyridium* sp.): α = 1.935 $\times 10^{-3}$ $\mu\mathrm{E}^{-1}\mathrm{m}^2$, β = 5.785 $\times 10^{-7}$ $\mu\mathrm{E}^{-1}\mathrm{m}^2$, γ = 1.460 $\times 10^{-1}\mathrm{s}^{-1}$, δ = 4.796 $\times 10^{-4}\mathrm{s}^{-1}$.

3.1. Preliminary assumptions

Generally speaking, the microalgal cells are solid particle and the CO_2 consumed and O_2 evolved are gases, thus we deal with the multiphase flow and transport. Nevertheless, the fluid flow will be treated as a flow of a ***suspension***. The continuous phase is the liquid medium (the gaseous phase is neglected) and the dispersed phase represents the microalgal cells. Although the cell morphology and cell size could be very diverse, we could state that the average diameter of a spherical microalgae is about ten micrometers.

Further, because *the mass fraction* of cells is low, the suspension is classified as *dilute* and Newtonian viscosity relationship is supposed. A. Richmond in [23] states that the least ultra-high cell density (UHCD) culture should have the dry weight biomass concentration of about 10 kg m^{-3}, which represents the 1 % mass fraction in the suspension of mass density about 1000 kg m^{-3}. The *volume fraction* of cells is similarly low (we assume that the cells are neutrally buoyant). Taking into account a uniform distribution of algal cells and the fact that the characteristic time of algal growth is in order of hours, we assume that mass density of the suspension (mixture) is $\rho = \rho_w$.

Thereafter, by virtue that the inter-particle distances in our case of dilute suspension are sufficiently large, the full flow field over each particle or cell is allowed to be developed. Consequently, the particle velocity differs from the fluid transport velocity only by the fact that the particle could be settling relatively to the fluid velocity in a direction parallel to gravity,[5] i.e. the microalgal cells follow the same trajectories as elementary fluid particles.[6]

3.2. Couette-Taylor fluid dynamic regimes

Couette-Taylor device is mainly composed of two coaxial cylinders. In our laboratory CTBR, the algal suspension in the annular space between cylinders is set in motion by the rotation of the inner cylinder ($r_i = 0.075$m) along the vertical axis, while the outer cylinder ($r_i = 0.1$m) is kept at rest. Several hydrodynamic regimes depend on an angular velocity Ω, on the geometrical characteristics of the device and on the physical properties of the fluid (kinematic viscosity ν).

According to Taylor's results [26], when the so-called Taylor number: $\mathrm{Ta} = \frac{(r_e - r_i)^3 r_i}{\nu^2}\Omega$, is smaller than a critical value (Ta_c), the flow in the system is purely tangential and is called the *Couette flow*. When the Taylor number is superior to this critical value, a transition to a periodic structure is observed. A series of toroidal vortices are superposed to the tangential flow, thus the *laminar Taylor vortex flow*, characterised by a laminar cellular vortex motion, occurs (see fig. 1). According to Taylor's explanation [26], the transition between the two regimes is achieved when the viscous forces do not damp the initial infinitesimal disturbances anymore, and this condition is reached when the Taylor number exceeds the given critical value. A further increase of the Taylor number leads to a sequence of two time-dependent flow regime, the *wavy vortex flow* and the *doubly periodic wavy vortex flow*.

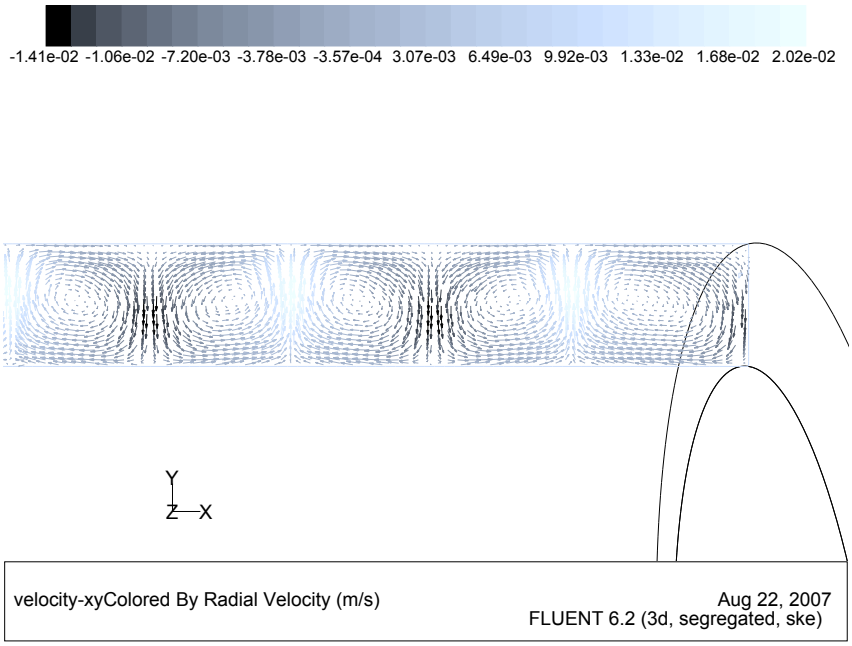

Fig. 1. Velocity profile in the axial section of the laboratory CTBR (for the inner cylinder angular frequency Ω = 1.5 rad s^{-1}), calculated by Fluent.

3.3. Methodology of the relative flow rates f_{ij} estimation

By definition, the term $f_{ij}S_{ij}$ (unit: m^{3}s^{-1}) represents the volumetric flow rate from compartment i to compartment j, see (3). When the total number of compartments is n_c, then the matrix of size $(n_c \times n_c)$ with elements f_{ij} can be constructed. Generally, the matrix is not symmetric when the convective transport is present. When the transport is carried out only by the dispersion, the corresponding matrix of coefficients f_{ij} is symmetric. In our case of Couette-Taylor bioreactor irradiated from outside, the surfaces S_{ij} are chosen as envelopes of coaxial cylinders. Then the coefficients f_{ij} will be determined from CFD numerical simulations based on our original method. The problem is divided into two parts:

- CFD simulation of particle trajectories by Fluent: The dispersion of particles was modelled using a stochastic discrete-particle approach, so-called Discrete Random Walk – DRW model (see fig. 2).

- Counting the number of particles crossing the border between adjacent compartments using MATLAB®: The coordinates of each of 7552 particles were post-processed using MATLAB®, and the dependency of the number of particles crossing the surface S_{ij} on time was drawn (see fig. 3). The values of flow rates f_{ij} are derived from the relation:

$$\frac{(\frac{N_{ij}{}^{+}}{S_{ij}})}{t} = \frac{N_T}{V}\, f_{ij}\,. \tag{9}$$

[5]Another effect should be taken into account while designing the bioreactors: biofouling by cell adhesion to the reactor walls.

[6]The same assumption was accepted by J. Pruvost *et al.* [22] arguing that the smallest eddy size, given by the Kolmogorov scale for their operating conditions, their annular PBR and their microorganism, is ca. ten times greater than the cell size.

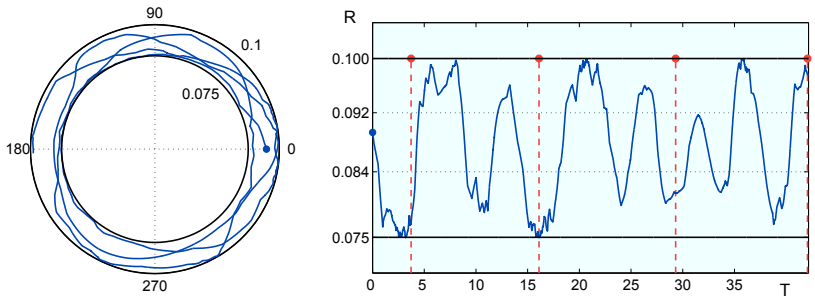

Fig. 2. Result of CFD simulation of one particle trajectory by Fluent. The particle trajectory in the CTBR cross-section is shown in the left side. The right-side picture describes the time course of the particle radial position.

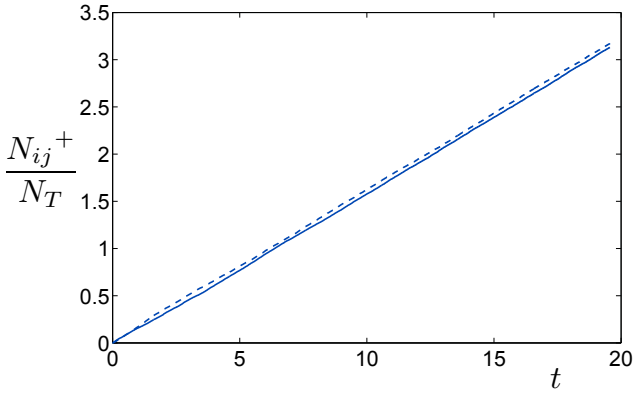

Fig. 3. Time course of the number of particles crossing the inter-compartment border (in both directions) divided by the total number of particles injected to the CTBR. The border was set as the envelope of the cylinder with radius r = 0,084 m.

The left side of (9) can be easily estimated from the fig. 3, where $N_{ij}{}^{+}$ means the number of particles crossing the $(i-j)-\mathrm{th}$ inter-compartment border, and N_T is the total number of particles injected to the CTBR.

Resuming: there is a numerical techniques to determine the coefficients f_{ij}. These coefficients are dependent on the CFD calculation inputs. Nevertheless, the number of these inputs is limited (for a given fluid and given CTBR geometry, it is only the angular velocity Ω). Therefore, the response-surface technique [12] looks promising. However, the detailed analysis is left for the near future.

4. Conclusion

The main purpose of this paper was to model the microalgal growth in Couette-Taylor photobioreactor in order to optimise either operating conditions and CTBR design. The unified modelling framework describing transport and photosynthetic reaction processes in CTBR was presented. The reason for using the hybrid multicompartment/CFD approach was explained: 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. 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 novel methodology for inter-compartment flow rates estimation based on the counting of number of particles crossing the border between adjacent compartments was introduced. The predicted microalgal cells trajectories within the vessel (computed by CFD program Fluent), reveals at the same time good (expected) qualitative properties and the "counting method" seems coherently (see fig. 3).

Our future goals are related to further experimental verification of the presented modelling framework and its application into a real PBR: (i) to prepare an experimental facility and test our method of inter-compartment flow rates estimation, (ii) to compare the behaviour of CTBR model and it of a real device (i.e., performing a growth experiment in a laboratory CTBR), and (iii) to apply (after having succeeded in the first two points) the multicompartment/CFD modelling approach to simulate the behaviour of our pilot PBR with Fresnel lenses [15].

Acknowledgements

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