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Abstract:

The development of a distributed parameter model of microalgae growth is presented. Two modelling frameworks for photo-bioreactor modelling, Eulerian and Lagrangian, are discussed and the complications residing in the multi-scale nature of transport and reaction phenomena are clarified. It is shown why is the mechanistic two time-scale model of photosynthetic factory the adequate model for biotechnological purposes. For a special laboratory Couette-Taylor bioreactor with cylindrical geometry, we reached a reliable simulation results using steady-state Eulerian approach and the finite difference scheme. Moreover, we prove numerically that the resulting photosynthetic production rate in this reactor goes, for growing inner cylinder angular velocity, to a certain limit value, which depends on the average irradiance only.

Keywords:

multi-scale modelling, distributed parameter system, boundary value problem, photosynthetic factory, photobioreactor

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1 Introduction

Biotechnology with microalgae and photo-bioreactor (PBR) design is nowadays regaining attention thanks to emerging projects of CO₂ sequestration and algae biofuels. Nevertheless, there neither exist reliable methods nor software for modelling, simulation and control of PBR [13]. Modelling in a predictive way the photosynthetic response in the three-dimensional flow field seems unrealistic today, because the global response depends on numerous interacting intracellular reactions, with various time-scales. In our previous works [9, 12, 10], we examined an adequate multi-scale lumped parameter model, describing well the principal physiological mechanisms in microalgae: photosynthetic light-dark reactions and photoinhibition. Now our main goal is the development and implementation of a mathematical model of microalgae growth in a general gas-liquid-solid PBR as tool in PBR design and optimization of its performance. Afterward, as a case study, we simulate the growth of microalgae in Couette-Taylor bioreactor [8], in order to validate our results.

2 Development of a distributed parameter model of microalgae growth in a PBR

Leaving apart the inherently non-reliable scale-up methodology for PBR design [13], two main approaches for transport and bioreaction processes modelling are usually chosen [14]: (i) Eulerian, and (ii) Lagrangian. While the Eulerian approach, resulting in partial differential equations, is a usual way to describe transport and reaction phenomena in bioreactors, the Lagrangian approach, leading either to stochastic ordinary differential equations or to random walk simulation of transport by turbulent diffusion (hydrodynamic dispersion), is an interesting alternative to PBR models.

Till nowadays, the most important information about the photosynthetic production of some microalgae species resides in the measurement of the coupling between photosynthesis and irradiance (being a controlled input), in form of the steady-state light response curve (so-called *P-I curve*), which represents the microbial kinetics, see e.g. *Monod* or more general *Haldane* type kinetics [14]. However, PBR operating under high irradiance, permitting large non-homogeneities of irradiance and allowing the photoinhibition of the cell culture and the photolimitation as well, belong to intensively studied topics of microalgal biotechnology, see e.g. [13] and references within there. Hence, we need such a model of microalgal growth, which can describe both the steady state and dynamic phenomena, i.e. it has to fulfill the following experimental observations: (i) the steady state kinetics is of *Haldane* type or *Substrate inhibition kinetics* [7]; (ii) the microalgal culture in suspension has the so-called *light integration* property [15, 7], i.e. as the light/dark cycle frequency is going to infinity, the value of the resulting production rate (e.g. oxygen evolution rate) goes to a certain limit value, which depends on the average irradiance only [9]. These features are best comprised by the mechanistic **model of photosynthetic factory** - PSF model [5, 16, 9]. Using the re-parametrization firstly introduced in [12], three-state PSF

model has the following form:

$$\dot{y} = [\mathcal{A} + u(t)\mathcal{B}] y, \quad \mu = q_2 q_3 y_A(t), \quad (1)$$

$$\mathcal{A} = q_4 \begin{bmatrix} 0 & q_2(1 + q_5) & \frac{q_5}{q_2(1+q_5)} \\ 0 & -q_2(1 + q_5) & 0 \\ 0 & 0 & -\frac{q_5}{q_2(1+q_5)} \end{bmatrix}, \quad \mathcal{B} = q_4 \begin{bmatrix} -1 & 0 & 0 \\ 1 & -q_5 & 0 \\ 0 & q_5 & 0 \end{bmatrix}, \quad (2)$$

where $y = (y_R, y_A, y_B)^\top$, $y_R + y_A + y_B = 1$, and q_i , $i = 1 \dots 5$, are five positive model parameters, cf. [12, 10]. Notice that the steady state PSF model behavior is defined by the parameters q_1, q_2, q_3 ($q_1 := I_{opt}$, I_{opt} maximizes μ), and the PSF model dynamics is determined by the *fast* rate q_4 and the *slow* rate $q_4 q_5$, for more details cf. [12, 10]. Notice also that (1) is composed by one ODE system and one algebraic equation connecting the hypothetical state y_A of PSF model with the specific growth rate $\mu := \dot{c}_x/c_x$, where c_x stands for microbial cell concentration. Considering that the value of q_3 is of order 10^{-4} s^{-1} , cf. [16], and $y_A(t)$ is periodic with period T , cf. [9] for more details, we have for the specific growth rate: $\mu = \frac{q_2 q_3}{T} \int_0^T y_A(t) dt$. PSF model successfully simulates the growth in high-frequency fluctuating light conditions because the growth is described through the "fast" state y_A , hence the sensitivity to high-frequency inputs, see e.g. flashing light experiments [7] or light/dark cycles induced by hydrodynamic mixing, is reached.

The single scalar input $u(t)$, representing the dimensionless irradiance in the culture, is defined as $u := I/q_1$, where I is the non-scaled irradiance (units: $\mu\text{E m}^{-2} \text{ s}^{-1}$). It is assumed that $u(t)$ is at least piecewise continuous. In other words, PSF model is the so-called bilinear controlled system which inherent property is the so-called light integration capacity [7], i.e. due to the *Lipschitz dependence of trajectories on control*, cf. [2] and references within there, as the frequency of fluctuating light is going to infinity, the value of resulting production rate (specific growth rate μ) goes to a certain limit value, which depends on average irradiance only [9]. For the constant input signal (irradiance $u \geq 0$) the ODE system (1) is linear and its system matrix $\mathcal{A} + u\mathcal{B}$ has three distinct eigenvalues. Two eigenvalues are negative (λ_F, λ_S), and the third is zero (its corresponding eigenvector is the globally stable steady state solution of (1)). In the sequel, we will need the steady state values of states y_A and y_B :

$$y_{A_{ss}} = \frac{u}{q_2(1 + q_5)(u^2 + u/q_2 + 1)}, \quad y_{B_{ss}} = \frac{u^2}{u^2 + u/q_2 + 1}. \quad (3)$$

Eq. (1) represents, for some known input signal $u(t)$, the **Lagrangian model of PBR**. However, it should be stressed that $u(t)$ is a random variable, depending on the fluid flow in PBR.

In some special, although common, conditions, e.g. in the case of constant average irradiance $u_{av} := \frac{1}{t_f - t_0} \int_{t_0}^{t_f} u(t) dt$, and when the period of light fluctuation is "small", we can simplify the ODE system (1) by reducing the PSF model dynamics to the one dimensional system using the singular perturbation approach with respect to the small parameter $q_5 \approx 10^{-4}$. The system (1) thanks to the properties of its right hand side clearly

satisfies the sufficient condition for the convergence of the singular perturbation [6]. One can therefore take the limit $q_5 \rightarrow 0$ in (1) to obtain:³

$$\dot{y}_A^F = -q_4 q_2 y_A^F + q_4 u(t) y_R, \quad \dot{y}_B^F = 0,$$

and consequently (recall that $y_R = 1 - [y_A + y_B]$):

$$\dot{y}_A^F = -q_4(u(t) + q_2)y_A^F + q_4 u(t) [1 - y_{B_{ss}}(u_{av})]. \quad (4)$$

3 Microalgae growth in Couette-Taylor bioreactor: Simulation results

We aim to simulate, eventually to optimize, microalgae cell growth in a Couette-Taylor bioreactor (CTBR) with cylindrical geometry, cf. [8]. For the sake of clarity, we further suppose all phenomena are axi-symmetrical, i.e. CTBR is homogeneously illuminated from the outside, and the biomass concentration is sufficiently high for making irradiance level decreasing from the CTBR outer wall to the CTBR core. Thus, the CTBR volume (our computational domain) can be divided into layers with the same irradiance level. Moreover, we also transform the 3D fluid dynamics problem into the one-dimensional. It means that only the cell motion in direction of light gradient is taken into account. Let then suppose this motion is caused by the turbulent diffusion (hydrodynamic dispersion) characterized by the dispersion coefficient $D_e(r)$, the tensor of second order in 3D case.

As stated before, the only input parameter determining the bio-reaction rate is the spatially dependent irradiance $u(r)$. Based on [4] we use the following relations for $u(r)$ and for the average (absorbed) irradiance:

$$u(r) = \frac{R}{r} \frac{u_1 \cosh \kappa \frac{r}{R}}{\sinh \kappa}, \quad u_{av} = u_1 \frac{2R^2}{R^2 - r_0^2} \frac{[\sinh \kappa - \sinh \kappa \frac{r}{R}]}{\kappa \cosh \kappa}, \quad (5)$$

where u_1 is the incident irradiance on the outer CTBR wall, κ is the dimensionless attenuation coefficient, R and r_0 are the outer and inner cylinder radii, respectively. The dimensionless attenuation coefficient $\kappa > 0$ is defined as follows: $\kappa := \frac{\ln(2)R}{r_{1/2}}$, where $r_{1/2}$, is the length interval (unit: m) making diminish the intensity of light to one half (in rectangular geometry). Furthermore, we introduce the dimensionless spatial coordinate in radial direction x , and dimensionless dispersion coefficient $p(x)$ as follows:

$$x := \frac{r}{R}, \quad x \in \left[\frac{r_0}{R}, 1 \right], \quad D_e := p(x)D_0, \quad p(x) := p_0 + p_1 [1 - (|2x - 1|)^n], \quad (6)$$

where D_0 is a constant with some characteristic value (unit: m^2s^{-1}), and p_0, p_1, n are dimensionless positive constants (to be determined empirically).

³Roughly speaking we can also apply the theorem of *Lipschitz dependence of trajectories on control* [2, 9, 10] when we suppose that the period of light cycles is "sufficiently small" for "averaging" of y_B but not so small for averaging y_A .

According to [1], nearly all mass transfer is linearly dependent on the driving force. Hence, for the growing power supply to the CTBR (by augmenting inner cylinder angular velocity ω) we expect D_0 proportionally grows, meanwhile the D_e shape, i.e. $p(x)$, remains constant. All the values needed to perform further calculations are summarized in Table 1 (u_1 is chosen accordingly to fulfill the condition $u_{av} = 1$):

u_1	D_0	κ	r_0	R	p_0	p_1	q_2	q_4	n
$\frac{R^2-r_0^2}{2R^2} \frac{\kappa \cosh \kappa}{[\sinh \kappa - \sinh \kappa \frac{r}{R}]}$	0.0001	$24 \ln(2)$	0.04	0.06	2	1	0.3	0.5	2

Table 1: Parameters summary

Similarly as in our work [11], Lagrangian time dependent simulation (data not shown) revealed that the state vector converges to a steady state in few minutes (this is the time scale of the photoinhibition process). Moreover, only the long term cultivation either in continuous or batch operation mode, where the quasi-steady state is reached, is of biotechnological importance. Consequently, based on the above reasons, our **Eulerian modelling approach** is simpler than generally three dimensional non-stationary transport-reaction PDE system:

$$\frac{\partial y}{\partial t} - \nabla \cdot (D_e(\vec{r}) \nabla y) = [\mathcal{A} + u(r)\mathcal{B}]y \quad \text{in } \Omega, \quad \nabla y = 0 \quad \text{on } \partial\Omega.$$

Furthermore, employing the fast reduction (4) and omitting the upper index "F",⁴ we get only one ODE for modelling the steady state of one state y_A in radial direction x (i.e. x is the only one independent variable):

$$-\frac{1}{x} [xp(x)y'_A]' + q(x) y_A = q(x) y_{A\infty}, \quad y'_A(r_0/R) = 0, \quad y'_A(1) = 0, \quad (7)$$

where $q(x) := \frac{q_4(u(x)+q_2) R^2}{D_0}$. The function $y_{A\infty}(x)$ is calculated as the steady state solution of (4):

$$y_{A\infty}(x) = \frac{u(x)}{u(x) + q_2} [1 - y_{Bss}(u_{av})] = \frac{u(x)}{u(x) + q_2} \left[\frac{u_{av} + q_2}{q_2(u_{av}^2 + u_{av}/q_2 + 1)} \right].$$

Let the characteristic number, the so-called *Damköhler number* of second type, be defined as $Da_{II} := \frac{q_4 R^2}{D_0}$, then $q(x) := (u(x) + q_2) Da_{II}$ holds. In the sequel, the dependence of the solution of (7) on Da_{II} will be studied.

The **boundary value problem** with Neumann boundary conditions and inhomogeneous right-hand side (7) has a lot of nice properties. It is symmetric and positive and the corresponding linear differential operator of the second order is self-adjoint. As $q(x) > 0$, problem (7) has a unique solution. It was solved numerically using the finite difference

⁴The lower index "ss" is omitted as well, nevertheless, when some confusion could arise, the term $y_A(x, \infty)$ is used.

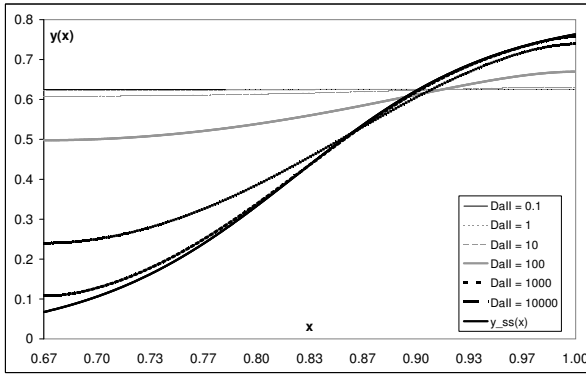


Figure 1: Approximate solution of (7): $y_A(x, \infty)$ vs. x .

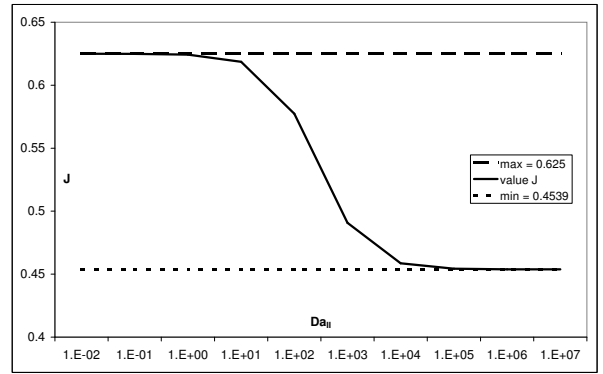


Figure 2: Performance index J vs. Da_{II} , cf. (8).

scheme for uniformly distributed nodes with the steplength h . It leads to the symmetric and positive definite system of linear equations with the tridiagonal matrix for unknown values

$$y_{A_i} = y_A(x_i) \equiv y_A(x_i, \infty), \quad i = 0, \dots, N.$$

The scheme approximates the exact solution of the boundary value problem (7) with accuracy of order h^2 .

In our numerical experiments we have chosen the values from Table 1 together with $N = 1000$. The following Fig. 1 shows the dependence of the solution on the *Damköhler number* Da_{II} . We can see that the solution approaches constant value $y_A(x, \infty) = 0.625$ for $Da_{II} \rightarrow 0$. Let us see that the solution becomes flatter for decreasing Da_{II} and for $Da_{II} = 0.1$ the solution is nearly constant. Notice also that the value $y_A = 0.625$ corresponds to the value $y_{A_{ss}}(1) = \frac{1}{2q_2+1}$, cf. (3). This means that the ODE system (7), for the case $Da_{II} \rightarrow 0$, performs the "averaging" of $u(x)$.

From practical point of view, in order to maximize the specific growth rate, cf. (1), it is important to evaluate the integral average of the activated state $y_A(x, \infty)$, depending on the operational conditions, i.e. on the u_1 and on ω . Let define

$$J = \frac{1}{V} \int_V y_A(x, \infty) dV = \frac{2}{R^2 - r_0^2} \int_{r_0/R}^1 xy_A(x, \infty) dx, \quad (8)$$

recalling that $y_A(x, \infty)$ is a solution of (7). Then we can formulate the optimization problem residing in maximizing of J . The next Fig. 2 shows the dependence of J , cf. (8), on Da_{II} , for the incident irradiance u_1 taken from Table 1. The maximum value arises for $Da_{II} \rightarrow 0$ and its value is again $J = 0.625$. The minimum value in (8) arises when the solution of (7) is $y_A(x, \infty) = y_{A_\infty}(x)$, which leads to a value $J \approx 0.4539$.

4 Conclusions

The main benefit of this paper resides in an extension of a multi-scale lumped parameter model of photosynthetic factory to the domain with heterogeneously distributed relevant parameters; in our case these parameters are irradiance and hydrodynamic dispersion (turbulent diffusion). For a special laboratory bioreactor based on Couette-Taylor flow, the so-called Couette-Taylor bioreactor, we reached reliable simulation results using Eulerian modelling framework and the finite difference scheme. Moreover, our results reflect well the dependence of microalgae growth on *Damköhler number* Da_{II} , i.e. on hydrodynamic dispersion (depending on inner cylinder angular velocity ω), permitting the announcement of our statement about *light integration property of PSF model* for CTBR as well: The resulting photosynthetic production rate in CTBR, for growing ω , goes to a certain limit value, which depends on the average irradiance only.

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