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Technical report No. 1112

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Abstract:

The paper deals with photosynthetic microorganism growth modelling and simulation in a distributed parameter system. Main result concerns the development and comparison of two modelling frameworks for photo-bioreactor modelling. The first "classical" approach is based on PDE (reaction-turbulent diffusion system) and finite difference method. The alternative approach is based on random walk model of transport by turbulent diffusion. The complications residing in modelling of multi-scale transport and reaction phenomena in microalgae are clarified and the solution is chosen. It consists on phenomenological state description of microbial culture by the lumped parameter model of photosynthetic factory (PSF model) in the re-parametrized form, published recently in this journal by Papáček, et al. (2009). Obviously both approaches lead to the same simulation results, nevertheless they provide different advantages.

Keywords:
multi-scale modelling, distributed parameter system, boundary value problem, random walk, photosynthetic factory.

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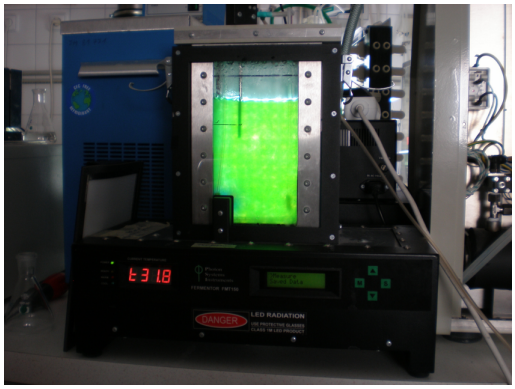
1 Introduction

The photosynthetic microorganism growth description is usually based on the microbial kinetics (so-called *P–I curve*), i.e. on the static lumped parameter models (LPM) describing the photosynthetic response in small cultivation systems with a homogeneous light distribution [5, 23]. However, there is an important phenomenon, which occurs under fluctuating light condition, the so-called flashing light enhancement, demanding 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, see e.g. [24]. Nevertheless, even having an adequate dynamical LPM of microorganism growth, e.g. phenomenological model of so-called photosynthetic factory [6, 7, 10, 27], another serious difficulty resides in the description of the microalgal growth in a photo-bioreactor, i.e. in a distributed parameter system with strongly non-homogeneous light distribution, e.g. accordingly to the exponential attenuation, see Section 4.

In our previous papers [16, 21, 18] we studied the PSF model behavior and the techniques for parameter estimation as well. In this paper we aim to develop the distributed parameter model (DPM) of a photosynthetic microorganism growth in a photo-bioreactor (PBR), mainly due to the necessity to evaluate the PBR performance and to optimize PBR operating conditions. Leaving apart the inherently non-reliable scale-up methodology for PBR design [8, 13], two main approaches for transport and bioreaction processes modelling are usually chosen [23]: (i) Eulerian, and (ii) Lagrangian. While the Eulerian approach, leading to the partial differential equations (PDE), is an usual way to describe transport and reaction systems, the Lagrangian approach, resulting either in a stochastic ordinary differential equations, or in the further described technique based on random walk simulation of transport by turbulent diffusion, is an interesting alternative to the PDE models.

The main purpose of this paper is to clarify how the PSF model can be advantageously used in DPM of microalgae growth in a general PBR. Hence, after having presented the main results concerning PSF model as LPM in Section 2, in Section 3 we present the development of two above mentioned modelling approaches. Section 4 is devoted to simulate PBR performance. As a case study we took the PBR with rectangular geometry, see e.g. the flat-panel PBR and FMT 150 in Fig. 1 (for more details cf. [12] and references within there), receiving the problem depending only on one space coordinate in direction of light gradient. This simplification permits to formulate and solve the simple optimization problem, having as result the incident irradiance maximizing the PBR productivity (Subsection 4.3). The simulation results and advantages of each approach, as well as outlooks for further research, are discussed in the final section.



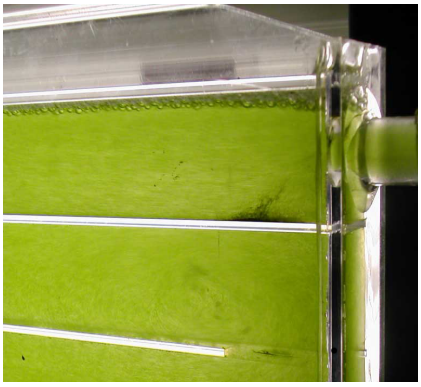


Figure 1: Two examples of rectangular PBR geometry: Photobioreactor FMT 150, made by Photon Systems Instruments, Czech Republic, www.psi.cz (left), and Flat panel photobioreactor, Institute of Physical Biology, University of South Bohemia, Nové Hrady, Czech Republic (right).

2 Lumped parameter model of photosynthesis and photoinhibition in microalgae

The dynamical **model of photosynthetic factory – PSF model**, see Fig. 2 below, has been thoroughly studied in the biotechnological literature [6, 7, 10, 27]. The state vector y of the PSF model is three dimensional, namely, $y = (y_R, y_A, y_B)^\top$, where y_R represents the probability that PSF is in the resting state R, y_A the probability that PSF is in the activated state A, and y_B the probability that PSF is in the inhibited state B. The PSF can only be in one of these states, so:

$$y_R + y_A + y_B = 1 \ . \tag{1}$$

The PSF model has to be completed by an equation connecting the hypothetical states of PSF model with some quantity related to the cell growth. This quantity is the specific growth rate μ. [3] According to [6, 27], the rate of photosynthetic production is proportional to the number of transitions from the activated to the resting state, i.e. $\gamma\ y_A(t)$. Hence, for the average specific growth rate we have the relation:

$$\mu = \frac{\kappa\gamma}{t_f - t_0} \int_{t_0}^{t_f} y_A(t)\mathrm{d}t \ , \tag{2}$$

where κ is a new dimensionless constant – the fifth PSF model parameter. Equation (2) reveals the reason why PSF model can successfully simulate the microalgae growth in high-frequency fluctuating light conditions: the growth is described through the "fast" state y_A, hence the sensitivity to high-frequency input fluctuations is reached, see e.g. flashing light experiments [15].

[3] $\mu := \dot{c}/c$, where c is the microbial cell density. The notation used is the most usual in biotechnological literature, cf. [5].

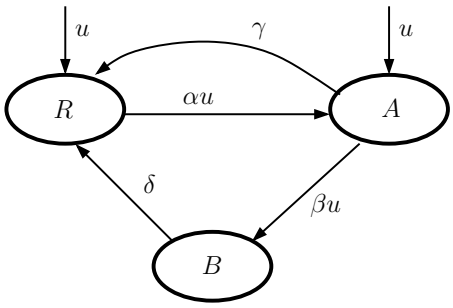


Figure 2: States and transition rates of the photosynthetic factory – Eilers and Peeters's PSF model.

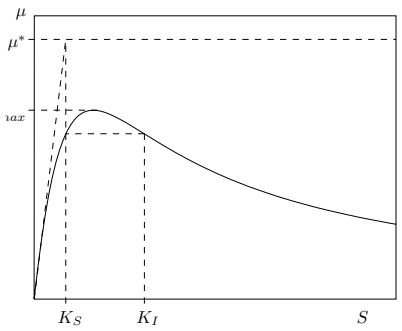


Figure 3: Steady-state production curve of *Haldane* type or *Substrate inhibition kinetics.* S stands here for irradiance.

2.1 Re-parametrization of the PSF model

Using the re-parametrization firstly introduced in [21], PSF model has the following form (recall that $y = (y_R, y_A, y_B)^\top$):

$$\dot{y} = \big[\mathcal{A} + u(t)\mathcal{B}\big]y, \tag{3}$$

$$\mathcal{A} = q_4 \begin{bmatrix} 0 & q_2(1+q_5) & \frac{q_5}{q_2(1+q_5)} \\ 0 & -q_2(1+q_5) & 0 \\ 0 & 0 & -\frac{q_5}{q_2(1+q_5)} \end{bmatrix}, \quad \mathcal{B} = q_4 \begin{bmatrix} -1 & 0 & 0 \\ 1 & -q_5 & 0 \\ 0 & q_5 & 0 \end{bmatrix}, \tag{4}$$

where the new parameters $q_i,\ i = 1, .., 5$, are relate to the old ones as follows:

$$q_1 := \sqrt{\frac{\gamma\delta}{\alpha\beta}}\,, \quad q_2 := \sqrt{\frac{\alpha\beta\gamma}{\delta(\alpha+\beta)^2}}\,, \quad q_3 := \kappa\gamma\sqrt{\frac{\alpha\delta}{\beta\gamma}}\,, \quad q_4 := \alpha q_1\,, \quad q_5 := \beta/\alpha\,. \tag{5}$$

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: μE m^{-2} 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 [15], i.e. due to the *Lipschitz dependence of trajectories on control*, cf. [4] 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 depend on average irradiance only [16].

Let us see that $q_1 = I_{opt}$ (I_{opt} maximizes μ, see Fig. 3 and Remark 1), q_2, q_5 are dimensionless, q_3, q_4 are in s^{-1}. The reasoning for such a choices arises from the utility to separate the steady state PSF model behavior (parameters q_1, q_2, q_3) from the PSF model dynamics (the *fast* rate $q_4 := \alpha I_{opt}$ and the *slow* rate $q_4 q_5 := \beta I_{opt}$), for more details cf. [21, 18]. The relation for the specific growth rate is now:

$$\mu = q_2 q_3 (1+q_5) \frac{1}{t_f - t_0} \int_{t_0}^{t_f} y_A(t)\mathrm{d}t\,. \tag{6}$$

For the constant input signal (irradiance $u \geq 0$) the ODE system (3) is linear and its system matrix $\mathcal{A} + u\mathcal{B}$ has three distinct eigenvalues. Two eigenvalues are negative ($\lambda_F,\ \lambda_S$), and the third is zero (its corresponding eigenvector is the globally stable steady state solution of (3)). In the sequel, we will need the steady state values of states y_A and y_B:

$$y_{A_{ss}} = \frac{u}{q_2(1+q_5)(u^2+u/q_2+1)}\ , \quad y_{B_{ss}} = \frac{u^2}{u^2+u/q_2+1}\ . \tag{7}$$

Remark 1: Notice that the parameter q_5 quantifies the separation between the fast and slow dynamic; $q_5 \approx 10^{-4}$, based on [27].[4] Moreover, the PSF model steady state behavior corresponds to *Haldane* type kinetics (or so-called *Substrate inhibition kinetics*), see Fig. 3: $\mu = \frac{\mu^*\ I}{K_S+I+I^2/K_I}$, where I is irradiance (i.e. limiting substrate S for photosynthetic microorganism) and $\mu^*,\ K_S,\ K_I$ are model constants. The connection between PSF model and *Haldane kinetics* could be described as follows: $\mu^* = q_2q_3$, $K_S = q_1q_2$, and $K_I = \frac{q_1}{q_2}$. For the constant value of irradiance which maximizes the steady-state growth rate, i.e. $I_{opt} := q_1 = \sqrt{K_SK_I}$, holds $\mu(I_{opt}) := \mu_{max} = \frac{\mu^*}{2\sqrt{K_S/K_I}+1} = \frac{q_2q_3}{2q_2+1}$. See also that for $K_I \to \infty$, the production curve changes to *Monod* kinetics.

2.2 Order reduction of the ODE system (3)

In some special although common conditions, e.g. in the case of constant average irradiance $u_{av} := \frac{1}{t_f-t_0}\int_{t_0}^{t_f} u(t)\mathrm{d}t$, and when the period of light fluctuation is "small", we can simplify the ODE system (3) by reducing the PSF model dynamics to the one dimensional one using the singular perturbation approach with respect to the small parameter $q_5 \approx 10^{-4}$ [25]. The system (3) thanks to the properties of its right hand side clearly satisfies the sufficient condition for the convergence of the singular perturbation. One can therefore take the limit $q_5 \to 0$ in (3) to obtain

$$\dot{y_A}^F = -q_4q_2\ {y_A}^F + q_4u(t)\ y_R\ , \quad \dot{y}_B^F = 0\ . \tag{8}$$

Upper index "F" aims to avoid confusion with notation for the non-reduced model (3). Taking into account the normalization condition (1), and preferring the states y_A, y_B (due to their measurability[5]), we further analyze only two above differential equations (8); for more detail see our paper [18]. The second relation in (8), i.e. $\dot{y}_B^F = 0$, means that the "slow" state variables reach its steady state value, i.e., $y_B = y_{B_{ss}}(u_{av})$. Recalling relation (1), i.e., $y_R = 1 - y_A - y_B$, only one ODE for the fast dynamics of ${y_A}^F$ state is received:

$$\dot{y_A}^F = -q_4(u(t)+q_2){y_A}^F + q_4u(t)\left[1 - y_{B_{ss}}(u_{av})\right]\ . \tag{9}$$

[4]For the microalga *Porphyridium* sp., on basis of Wu and Merchuk's parameters α, β, γ, δ, κ, we have calculated: $q_1 = 250.106\ \mu\mathrm{E\ m^{-2}}$, $q_2 = 0.301591$, $q_3 = 0.176498e-3\ \mathrm{s^{-1}}$, $q_4 = 0.483955\ \mathrm{s^{-1}}$, $q_5 = 0.298966e-3$.

[5]The connection of y_A with a measurable quantity describes (6), and y_B can be estimate via chlorophyll fluorescence measurement, cf. [12, 27].

Roughly speaking we can also apply the theorem of *Lipschitz dependence of trajectories on control* [4, 16, 18] 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. Further we denote the steady state solution of the above equation (9) as: y_{A_∞}. In subsection 4.3, we shall advantageously use this term.

3 Distributed parameter model of photosynthesis and photoinhibition in microalgae

Two approaches for modelling of microbial growth are usually chosen: (i) Eulerian, and (ii) Lagrangian. The first "more classical" approach, based on the balance equation for an infinitesimal volume, leads to the partial differential equation (reaction-convection-diffusion system). The quantities to describe are concentrations of microbial cells and some other species.

The Lagrangian approach, consisting in description of each individual microbial cell, offers two possibilities: first, to compute or measure (cf. e.g. [11]) the cell trajectories in PBR and evaluate the so-called irradiance history $u(t)$ as the stochastic input variable for the ODE (3), resulting in a stochastic ordinary differential equation; the second possibility is based on random walk simulation of transport by turbulent diffusion, and is further described in subsection 3.2.

3.1 Distributed parameter model of photosynthesis and photoinhibition in microalgae: Eulerian approach

Accordingly to [1], the transport and reaction phenomena of some species or components describes the following equation (where $c_i = c_i(\vec{r}, t)$ is either a species concentration or cell density):

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\vec{v} c_i) - \nabla \cdot (D_e \nabla c_i) = R \ , \quad i = 1, ..., m, \tag{10}$$

where R is the reaction (source) term, $\vec{v}$ is the velocity flow field, and $\vec{r}$ stands for a vector of space coordinates. $D_e(\vec{r})$ is the dispersion coefficient (generally the tensor of second order), which corresponds to the 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 (this explains why D_e is spatially dependent). 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 initial condition and boundary condition (impermeability of PBR walls, i.e. domain boundary ∂V) to (10) are following:

$$c_{i_0} = c_i(\vec{r}, t_0) \ , \quad \nabla c_i(\partial V, t) = 0, \quad i = 1, ..., m. \tag{11}$$

The solution of transport equation (10-11) usually causes many complications residing in fact that the relevant transport and reaction phenomena are multi-scale. If we realize

that the characteristic time of microalgae growth (e.g. doubling time $t_g := \frac{ln(2)}{\mu}$) is in order of hours, and the the characteristic time of turbulent diffusion ($t_d := \frac{L^2}{D_e}$) is in order of seconds (similarly that of convective transport $t_c := \frac{L}{v}$), then actually only two alternatives exist: (i) to neglect the details concerning mixing phenomena, e.g. by accepting the hypothesis that the entire cell culture dispersed in medium was homogenized at each calculation step (cf. [14], where the time step Δt was set to one hour), and (ii) to observe the changes due to the hydrodynamic mixing and neglect those of biochemical reaction. Both alternatives completely lose the coupling between transport and reaction phenomena, which qualify the corresponding modelling framework as unsatisfactory.

Our proposition to resolve about mentioned difficulties is based on the extension of PSF model "into space". The stochastic formulation of PSF model, as described in Section 2, is not unique: instead of one photosynthetic factory (with three states), we can imagine as many factories as cells in the cultivation system (i.e. PBR). Each microalgae cell with certain probability stays in its current state or is transformed into one of the remaining states, and at he same time it travels inside the PBR. Assuming we know the irradiance distribution in PBR, i.e. $u = u(\vec{r}, t)$, then we evaluate the specific growth rate not only as the value proportional to the temporal average of the activate state, cf. (6), but also the spatial averaging takes place:

$$\mu = q_2 q_3 (1 + q_5) \frac{1}{t_f - t_0} \int_{t_0}^{t_f} \left(\frac{1}{V} \int_V y_A(\vec{r}, t) \mathrm{d}V \right) \mathrm{d}t \ . \tag{12}$$

The only thing which rests to explain is how to introduce into the transport equation (10) the reaction term coherently with PSF model. Let us evaluate the PSF model states as relative concentrations (molar fractions) of microbial cells in respective state (R, A, or B). Let define the variables c_i as the concentrations of cells in respective states of PSF model, and c as an overall cell concentration. The concentrations are generally varying in time and space $c_i = c_i(x, t),\ i \in \{R, A, B\}$, nevertheless it holds: $c = c_R + c_A + c_B$. Consequently, without loss of precision, we re-define the state vector of PSF model as follows:

$$y = (y_R, y_A, y_B)^\top := \frac{1}{c} \ (c_R, c_A, c_B)^\top . \tag{13}$$

Furthermore, after dividing (10) by c, we can substitute the right hand side of PSF model equation (3) as the reaction term in the right hand side of the following (14):

$$\frac{\partial y}{\partial t} + \nabla \cdot (\vec{v} y) - \nabla \cdot (D_e \nabla y) = \big[\mathcal{A} + u(\vec{r}, t) \mathcal{B} \big] y \ . \tag{14}$$

Equation (14) with the corresponding initial and boundary condition (11) represents the PDE based model for describing multi-scale transport and reaction phenomena in a general PBR. To illustrate the reliability of our approach, we will analyze in Section 4, as a case study, the microalgae growth in a simple rectangular PBR.

3.2 Distributed parameter model of photosynthesis and photoinhibition in microalgae: Lagrangian approach

In our Lagrangian based modelling approach, both the biochemical reaction and transport are treated in a stochastic manner. This brings several advantages over the classical PDE based approach, high potential of parallel implementation, as described further, being one of them. Stochastic model of the transport is based on a discrete random walk model which reflects the spatially dependent turbulent diffusion coefficient. It is this coefficient that binds the stochastic behavior to the real hydrodynamic conditions in the simulated domain. Spatial dependence of the diffusion coefficient may be obtained by classical means, i.e. CFD (Computational Fluid Dynamics) numerical simulation for the given geometry. With respect to the implementation - mainly computational issues, the apparent advantage of this approach is mutual independence of the individual cells under cultivation, where every cell is represented by an independent photosynthetic factory, whose only input parameter is spatially dependent irradiance $u(\vec{r})$ (the temporal variation of irradiance is neglected, because it occurs in several order slower time-scale). The succession of states of the individual cells (R, A, and B) forms a Markov chain, with $\mathcal{A} + u\mathcal{B}$ being the system matrix of (3), the infinitesimal generator, see e.g. [3] and references within there. The details about algorithm design and implementation are discussed in the following Section 4.

4 Simulation results: Random walk vs. Finite difference method

4.1 Problem formulation

We aim to simulate, eventually to optimize microalgae cell growth in a PBR. For the sake of clarity, we further suppose the rectangular, axi-symmetrical PBR geometry, illuminated from one side, i.e. the irradiance level is decreasing from the PBR wall to PBR core, cf. Fig. 1. Thus, the PBR volume (our computational domain) can be divided into layers with the same irradiance level. Moreover, if the flow field in the PBR is stationary and does not depend on the coordinates perpendicular to the direction of light gradient, then we can neglect the cell motion over the layers with the same irradiance level, transforming the 3D problem into the one-dimensional. It means that only the cell motion in direction of light gradient is of most interest. This motion is caused by the turbulent diffusion (hydrodynamic dispersion) characterized by an only parameter $D_e(r)$, i.e. by the dispersion coefficient (a tensor of second order in 3D case).

As stated before, the only input parameter determining the bio-reaction rate is the spatially dependent irradiance $u(r)$. Here we announce the exponential, so-called Lambert-Beer law, and the relation for average (absorbed) irradiance, in the form:

$$u(r) = u_0 \; e^{-\Lambda r} \;, \quad u_{av} = u_0 \frac{1 - e^{-\Lambda L}}{\Lambda L} \;, \tag{15}$$

where u_0 is the incident irradiance, Λ is the attenuation coefficient (unit: m^{-1}) and L is the PBR thickness in direction of light gradient. It is convenient to define a dimensionless

"thickness constant" $k > 0$ as follows: $L := k\, r_{1/2}$, where $r_{1/2} := \frac{\ln(2)}{\Lambda}$, is the length interval (unit: m) making diminish the intensity of light to one half. Furthermore, we introduce the dimensionless spatial coordinate x as follows:

$$x := \frac{r}{L} , \quad x \in [0, 1] . \tag{16}$$

After this transform, we introduce also the dimensionless dispersion coefficient $p(x)$ by $D_e := p(x)\ D_0$, where D_0 is a constant with some characteristic value, unit: $\mathrm{m^2 s^{-1}}$. According to [1], nearly all physical exchange is linearly dependent on the driving force. Hence, for the growing power supply to the PBR pumping device we expect D_0 proportionally grows, meanwhile the D_e shape (i.e. $p(x)$) remains constant. For $p(x)$ we propose the following relation:

$$p(x) := p_0 + p_1 \left[1 - (|2x - 1|)^n\right] , \tag{17}$$

where p_0, p_1, n are dimensionless positive constants (to be determined empirically).

All the values needed to perform further calculations are summarized in Table 1:

u_0	D_0	k	L	p_0	p_1	q_2	q_4	n	$y_R(t_0)$	$y_A(t_0)$	$y_B(t_0)$
$\frac{8\ln(2)}{1-2^{-8}}$	0.0001	8	0.02	2	1	0.3	0.5	2	1	0	0

Table 1: Parameters summary

The values representing initial guess for operating conditions (to be optimized) are in the first two columns, the middle seven data are empirical constants, and the last three values are initial conditions for simulation of time course of PSF states. It is important at this stage to point out that the empirical data have an illustrative and testing purpose only.

4.2 Lagrangian simulation

The Lagrangian simulation algorithm was designed with parallel platform implementation in mind and was performed both on the classical PC and a parallel platform - namely CUDA (Compute Unified Device Architecture) architecture. Random walk model was implemented on top of the Mersenne Twister parallel random number generator in combination with Box-Muller transformation. With this parallel reimplementation on CUDA we were able to get an additional 90-fold gain in speed when compared to the single threaded implementation running on PC.

The simulation results for the Lagrangian simulation are summarized in Tables 2 and 3. From the last columns it is evident that the steady state was reached. All the simulation parameters besides D_0 were the same as shown in Table 1. The particular value $D_0 = 0.5$ was found empirically as a minimal D_0 at which the culture growth is not transport-limited, i.e. the mixing is sufficient.

Time [s]	0	1	10	50	100	500	1000	2000	3000	4000	5000
$y_{R_{av}}$	1.00	0.61	0.21	0.20	0.21	0.20	0.20	0.18	0.17	0.17	0.17
$y_{A_{av}}$	0.00	0.39	0.79	0.79	0.78	0.74	0.70	0.66	0.65	0.62	0.62
$y_{B_{av}}$	0.00	0.00	0.00	1.00	0.01	0.06	0.10	0.16	0.18	0.21	0.21

Table 2: Random walk simulation results, $D_0 = 0.5$, maximum growth rate reached

Time [s]	0	50	100	500	1000	2000	3000	4000	5000	10000
$y_{R_{av}}$	1.00	0.43	0.42	0.40	0.38	0.36	0.34	0.33	0.33	0.33
$y_{A_{av}}$	0.00	0.57	0.56	0.54	0.51	0.47	0.46	0.45	0.44	0.44
$y_{B_{av}}$	0.00	0.00	0.02	0.06	0.11	0.17	0.20	0.22	0.23	0.23

Table 3: Random walk simulation results, $D_0 = 0.005$

4.3 Eulerian simulation and optimization of incident irradiance u_0

Based on the previous time dependent Lagrangian simulation results, we argue that all PSF states are approaching some value $y_{i_{ss}}(x) = \lim_{t\to\infty} y_i(x,t),\ i \in \{R, A, B\}$, depending on the external inputs u_0 and D_0 only. Moreover, the inhibited state $y_{B_{ss}}(x)$ is nearly constant across the PBR (data not shown) and holds: $y_B = y_{B_{ss}}(u_{av})$.

Consequently, based on the above reasons, we modify the transport-reaction system (14) as follows: first, let put $\frac{\partial c}{\partial t} = 0$, then employ (9). We obtain (omitting the upper index "F"):

$$-\left[p(x)y_A'\right]' + q(x)\ y_A = q(x)\ y_{A_\infty}\ , \quad y_A'(0) = 0\ , \quad y_A'(1) = 0\ , \tag{18}$$

where

$$q(x) := \frac{q_4\,(u(x) + q_2)\ \ L^2}{D_0}.$$

The function $y_{A_\infty}(x)$ is calculated as the steady state solution of (9):

$$y_{A_\infty}(x) = \frac{u(x)}{u(x) + q_2}\left[1 - y_{B_{ss}}(u_{av})\right] = \frac{u(x)}{u(x) + q_2}\left[\frac{u_{av} + q_2}{q_2({u_{av}}^2 + u_{av}/q_2 + 1)}\right]. \tag{19}$$

Let the characteristic number, the so-called *Damköhler number* of second type be defined as

$$Da_{II} := \frac{q_4\ L^2}{D_0}, \tag{20}$$

then $q(x) := (u(x) + q_2)\ Da_{II}$ holds. Further, the dependence of the solution of (18) on Da_{II} will be studied.

The boundary value problem with Neumann initial conditions and inhomogeneous right-hand side (18) has a lot of nice properties. It is symmetric and positive and the corresponding linear differential operator of the second order

$$L(y_A) = -\left[p(x)y_A'\right]' + q(x)\ y_A,$$

is self-adjoint. As $q(x) > 0$, problem (18) has a unique solution (see e.g. [22], [26]). It was solved numerically using a following finite difference scheme with uniformly distributed nodes which leads to a symmetric and positive definite system of linear equations for unknown values

$$y_{Ai} = y_A(x_i) \equiv y_A(x_i, \infty), \quad i = 0, \ldots, N,$$

with a tridiagonal matrix:

$$\begin{pmatrix} a_0 & b_0 & 0 & \ldots & 0 \\ b_0 & a_1 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & b_{N-1} \\ 0 & \ldots & 0 & b_{N-1} & a_N \end{pmatrix} \begin{pmatrix} y_{A0} \\ \vdots \\ \vdots \\ \vdots \\ y_{AN} \end{pmatrix} = \begin{pmatrix} g_0 \\ \vdots \\ \vdots \\ \vdots \\ g_N \end{pmatrix}$$

where

$$\begin{aligned} a_0 &= p(x_0 + h/2) + h^2 q(x_0)/2, \\ a_i &= p(x_i - h/2) + p(x_i + h/2) + h^2 q(x_i), \quad i = 1, \ldots, N-1, \\ a_n &= p(x_N - h/2) + h^2 q(x_N)/2, \\ b_i &= -p(x_i + h/2), \quad i = 0, \ldots, N-1, \\ g_0 &= h^2 f(x_0)/2, \\ g_i &= h^2 f(x_i), \quad i = 1, \ldots, N-1, \\ g_n &= h^2 f(x_N)/2. \end{aligned}$$

Here $f(x) = q(x)\ y_{A_\infty}(x)$, $x_i = ih$, and $h = \frac{1}{N}$ where N denotes the number of nodes. Such a scheme approximates the exact solution of the boundary value problem (18) 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. 4 shows dependence of the solution on the *Damköhler number* Da_{II}. We can see that the solution approaches a constant value $y_A(x, \infty) = 0.625$ for $Da_{II} \to 0$. Let us see that the solution becomes flatter for decreasing Da_{II} and for $Da_{II} = 0.2$ the solution is nearly constant.

Now we can formulate the optimization problem residing in maximizing the integral average of the activated state $y_A(x, \infty)$, i.e., we aim to maximize the integral

$$J = \int_0^1 y_A(x, \infty) \mathrm{d}x. \tag{21}$$

recalling that $y_A(x, \infty)$ is a solution of (18).

The next Fig. 5 shows dependence of J on Da_{II}, for the incident irradiance u_0 taken from Table 1. The maximum value arises for $Da_{II} \to 0$ and its value is $J = 0.625$. Minimum value in (21) arises when the solution of (18) is $y_A(x, \infty) = y_{A_\infty}(x)$, which leads to a value $J \approx 0.4254$.

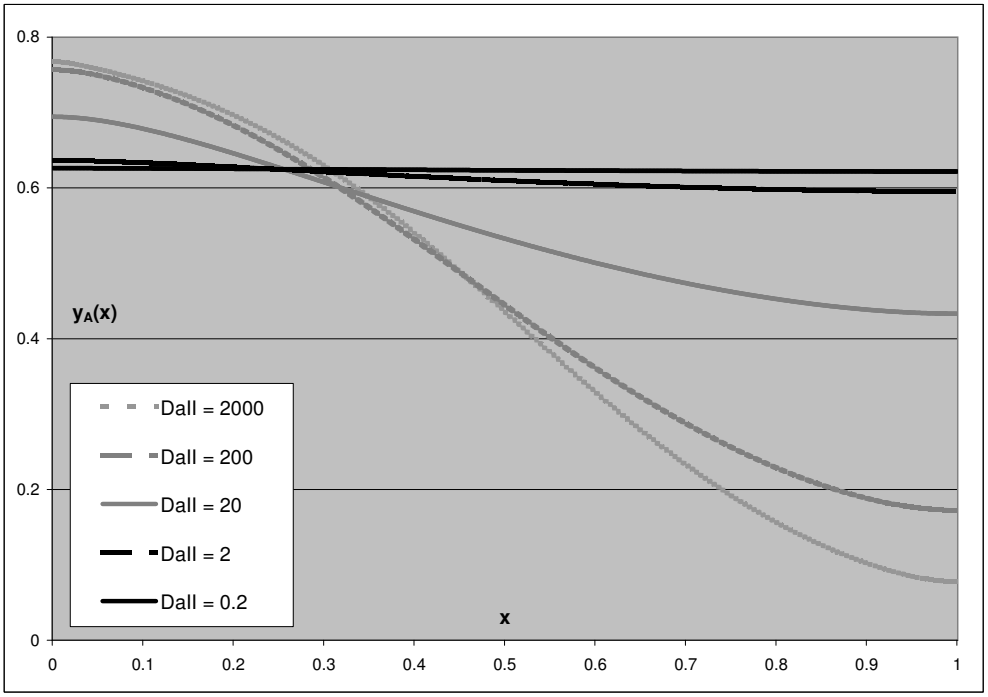


Figure 4: Approximate solution of (18)

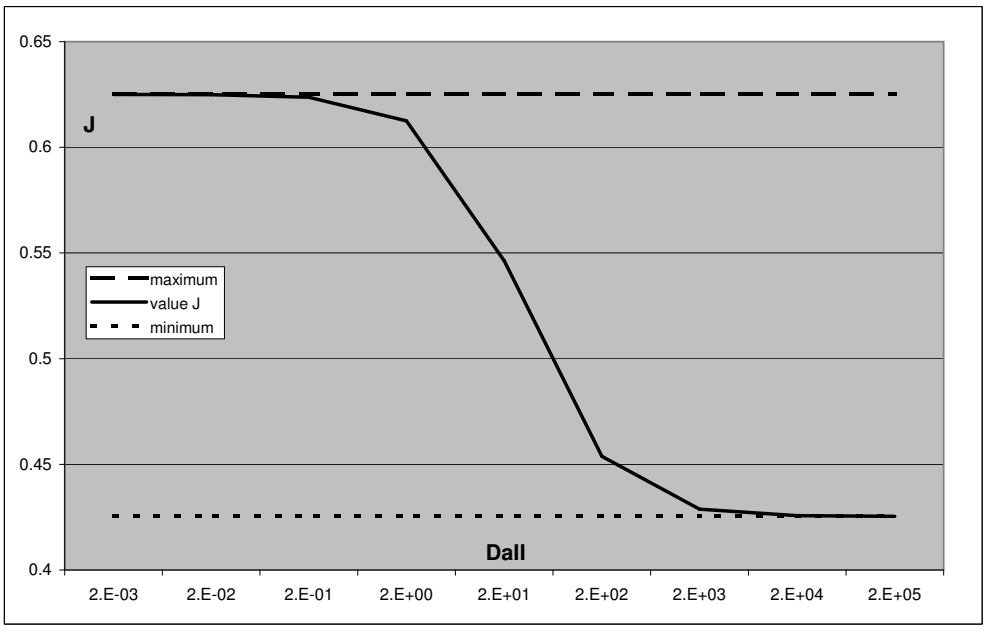


Figure 5: Value J

Remark 2: Notice that the value $J = 0.625$ corresponds to the value $y_{A_{ss}}(1) = \frac{1}{2q_2+1}$, cf. (7). This means that the ODE system (18), for the case $Da_{II} \to 0$, performs the "averaging" of $u(x)$.

We have made several simulations for various u_0 and the values of J were smaller than that for u_0 taken from Table 1. This is a numerical confirmation of the hypothesis often mentioned in biotechnological literature.

5 Asymptotic properties of the reaction-diffusion system (18)

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, 19]. 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 (18). Realizing that it was impossible, we did not search the solution in the usual form of $y = y(x)$ (here, for the simplicity, we omit the lower index A), 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 [26], the boundary value problem (18) 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

$$\frac{\mathrm{d}}{\mathrm{d}x}y = z\ , \quad \frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)z\right] = q(x)\ (y - y_{ss})\ , \quad z(0) = 0\ , \quad z(1) = 0\ . \tag{22}$$

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 (22) on $Da_{II} := \varepsilon \to 0$ could be studied.

The following ODE

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

thanks to the properties of its right hand side clearly satisfies the sufficient condition for applying the averaging method [9]. One can therefore approximate (22) as follows (always when $\varepsilon \to 0$):

$$\frac{\mathrm{d}}{\mathrm{d}x}y = z\ , \quad \frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)z\right] = \varepsilon \int_0^1 \left[k_A(u(x))\ (y - y_{ss})\right] \mathrm{d}x\ , \quad z(0) = 0\ , \quad z(1) = 0\ . \tag{23}$$

6 Conclusions

The purpose of this paper was to present an extension of a lumped parameter model of photosynthetic microorganism growth to the domain with heterogeneously distributed relevant parameters, e.g. irradiance and turbulent diffusion (hydrodynamic dispersion). The principal problem was to find how to reconcile the multi-scale problem in such a manner, that the corresponding modelling framework was sensitive to all relevant phenomena. The key decision was to adopt the model of photosynthetic factory (PSF model), which operates in three time-scales, being sensitive to the time-scale of turbulent diffusion.

Both approaches and corresponding numerical techniques, i.e. random walk and finite difference method, show the consistent results, proving the viability of our efforts. The advantage of the stationary PDE based model resides in less computationally expensive solution of optimization of PBR operating conditions.

On the other hand, Lagrangian approach and random walk technique permits the parallel stochastic simulation of microalgal growth in a real time.

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