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Lattice Boltzmann Methode zur Simulation des Strahlungstransports in Mikroalgen-Biosuspensionen

Lattice Boltzmann Method for the Simulation of Radiation Transport in Microalgae Biosuspensions

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Abstract

To optimize the cultivation of phototroph microorganisms, an accurate prediction of light intensity in photobioreactors is required. For this task, numerical simulation of radiative transfer necessitates an efficient coupling to flow solvers, since the optical properties of the cultivation broth depend on local concentrations of cells and gas bubbles. Based on recent developments, in this paper a lattice Boltzmann framework for radiative transfer is derived and validated against Monte Carlo simulations. Finally, the model is applied to predict the attenuation of light in a microalgae biosuspension.

Introduction

The technical cultivation of phototroph microorganisms, such as microalgae, depends on an efficient supply of light in photobioreactors. While insufficient supply of light limits cell growth, high light intensities lead to inefficient metabolic utilization of the supplied radiative energy or even may cause inhibition of growth (Torzillo & Vonshak 2013). Since light is usually considered to be the growth-limiting factor in full scale cultivation plants, the optimization of culture conditions has to take radiative transport and local light intensities into account. In photobioreactors, the solution of the radiative field is connected to the flow field inside the reactor because optical properties of the biosuspension depend on local concentrations of cells and gas bubbles, which are usually non-homogenously distributed. Due to the need of a detailed prediction of the spatial radiative field, recently the Radiative Transfer Equation (RTE) was used instead of the one-dimensional Lambert's Law to model radiative transfer in homogenous biosuspensions (Kong & Vigil 2014). To solve the RTE, different numerical methods, such as Discrete Ordinate Methods or Monte Carlo Methods, can be applied (Modest 2013). However, these methods cause either high computational costs or require different numerical grids from those used in Computational Fluid Dynamics. Thus, the interpolation of information between the different numerical grids becomes a necessity for the determination of local optical properties of biosuspensions. More recently, new approaches based on lattice Boltzmann methods were developed to solve the RTE in one and two dimensions (Asinari et

al. 2010, Ma et al. 2011, Di Rienzo et al. 2011, Bindra & Patil 2012). Since lattice Boltzmann methods are already applied successfully in Computational Fluid Dynamics, their application to radiative transfer seems to be promising to solve coupled radiation-flow problems on the same numerical grid with high accuracy. In this paper, a lattice Boltzmann framework for the simulation of radiative transfer is developed and applied to predict the three-dimensional steady-state distribution of monochromatic light in a homogenous microalgae biosuspension.

Lattice Boltzmann Modeling of Radiative Transport in Participating Media

The propagation of thermal radiative energy in participating media is affected by absorption, scattering and emission of radiation inside the medium. A common approach to predict radiative fields is to balance the radiative intensity I with respect to location $\vec{r}$, direction of propagation $\vec{s}$ and time t (Modest 2013). Moreover, the interaction of radiation with the medium depends on the frequency ν of the electromagnetic wave, and thus the balance equation becomes a seven-dimensional problem. By introducing the specific intensity I_ν and assuming steady-state of the radiative field, the RTE for an absorbing, emitting and scattering medium reads as follows.

$$\vec{s}\,\nabla I_\nu(\vec{r},\vec{s}) = \kappa_\nu I_{b,\nu} - \beta_\nu I_\nu(\vec{r},\vec{s}) + \frac{\sigma_\nu}{4\pi}\int_{4\pi} I_\nu(\vec{r},\vec{s}')\Phi(\vec{s}',\vec{s})d\Omega \qquad (1)$$

On the right-hand side of Eq. (1), the first term gives the emissivity of the medium, while the second term is the attenuation of intensity due to extinction. The extinction coefficient β_ν is related to the absorption coefficient κ_ν and the scattering coefficient σ_ν by the relation $\beta_\nu = \kappa_\nu + \sigma_\nu$. The third term denotes the in-scattering of radiation in the balanced direction $\vec{s}$ from directions $\vec{s}$' within the solid angle $d\Omega$ as described by the scattering phase function $\Phi(\vec{s}',\vec{s})$.

By considering the specific intensity as flux of photons with at given frequency, the RTE can be derived directly from the Boltzmann equation (Bodenheimer et al. 2006). Thus, a lattice Boltzmann approach to simulate radiative transfer seems to be a natural choice. According to the pioneer work of Ma et al. (2011), the discretized radiative transfer equation in an absorbing and emitting but non-scattering medium can be written in lattice Boltzmann terminology as follows.

$$\begin{aligned} I_{\nu,\vec{s}}(\vec{r}+c_{\vec{s}}\Delta t, t+\Delta t) - I_{\nu,\vec{s}}(\vec{r},t) = &-\frac{1}{\tau}\Big(I_{\nu,\vec{s}}(\vec{r},t) - I^{eq}_{\nu,\vec{s}}(\vec{r},t)\Big) \\ &+S_{\nu,\vec{s}}(\vec{r},t)\Delta t - c_{\vec{s}}\kappa_\nu I_{\nu,\vec{s}}(\vec{r},t)\Delta t \end{aligned} \qquad (2)$$

In Eq. (2), $S_{\nu,\vec{s}}$ is the emission source term and $c_{\vec{s}}$ is the speed of photon propagation in direction $\vec{s}$ on the lattice. The first term on the right-hand side is the collision term, which is applied to model particle-particle interactions. In contrast, Asinari et al. (2010) modeled a collision term to introduce isotropic scattering by considering scattering as collision with matter. Referring to both approaches, Bindra and Patil (2012) have shown that interparticle collisions of photons are neglectable. In addition, they replaced the scattering term as modeled by Asinari et al. (2010) by a simple source term and showed its applicability even to non-isotropic scattering in two dimensions. The resulting model equation contains an additional scattering-source term, where a quadrature formula replaces the in-scattering integral given by Eq. (1).

$$\begin{aligned} &I_{\nu,\vec{s}}(\vec{r}+c_{\vec{s}}\Delta t, t+\Delta t) - I_{\nu,\vec{s}}(\vec{r},t) \\ &\qquad = S_{\nu,\vec{s}}(\vec{r},t)\Delta t - c_{\vec{s}}\beta_\nu I_{\nu,\vec{s}}(\vec{r},t)\Delta t + \sigma_\nu c_{\vec{s}}\sum_{M} w_{\vec{s}'} I_{\nu,\vec{s}'}(\vec{r},t)\,\Phi(\vec{s}',\vec{s})\Delta t \end{aligned} \qquad (3)$$

In the next section, a lattice Boltzmann framework based on the model of Bindra and Patil is developed to reach a general model for more advanced velocity sets in three spatial dimensions.

Lattice Boltzmann Framework for the 3D Simulation of Radiative Transport

A suspension of photosynthetic active microorganisms, such as microalgae, can be considered to be an absorbing and scattering medium. In contrast to abiotic matter, those microorganisms do not, or only to a small extent, emit absorbed energy, since the energy is used for metabolic reactions. Thus, emission of radiative energy will be neglected in the following.
The formulation given by Eq. (3) is already discretized in space, direction, time and frequency and the full model contains one balance equation for each of the M discrete directions under consideration. In the cubic lattice, directions are defined by the connection between two lattice nodes as shown in Figure 1. In addition to the velocity sets shown, in this work D3Q50 and D3Q98 sets are used, which allow photons to propagate in the next outer belt and thus, increasing the angular resolution. It is important to state that the cubic nature of the lattice makes photons to travel different distances within one time step. Thus, the speed of photons depends on the direction of propagation which is not in accordance with the physics of light. Consequently, the model is restricted to the prediction of steady-state fields of specific intensity. However, the timescale of light propagation is much faster compared to timescales of cell movement in the flow or cell growth, which both result in changes of local optical properties.

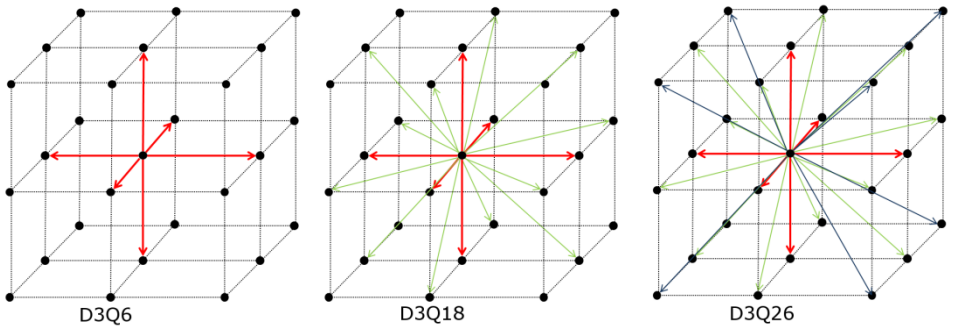

Figure 1: Examples of velocity sets applied for the simulation of radiative transfer.

To solve the in-scattering term it is necessary to determine the direction-associated quadrature weights, which are a measure of the solid angle related to each discrete direction. Following Huygens principle, every point along a wavefront can be considered as a source point of a new wave. Accordingly, every node in the lattice can be regarded to be a point source of electromagnetic waves. The electromagnetic wave propagates uniformly and the same amount of energy is emitted in every direction. Considering emitted energy as the emitted number of photons dN, the quadrature weight measures the fraction of photons emitted in a certain direction.

$$dE_{\vec{s}} \propto dN_{\vec{s}} = N_0 w_{\vec{s}} \tag{4}$$

Consequently, every direction has an equal quadrature weight. Conservation of energy requires

$$\sum_M w_{\vec{s}} = 1. \tag{5}$$

Specific Intensity is defined as monochromatic radiative power per solid angle, which is related to the photon flux dN/dt into this solid angle. Using the definition $d\Omega = 4\pi|\vec{r}|^2 w_{\vec{s}}$, the following expression can be obtained, where h is the Planck constant.

$$I_{\nu,\vec{s}} = h\nu \frac{dN}{dt}\frac{1}{d\Omega} = h\nu \frac{N_0 w_{\vec{s}}}{dt}\frac{1}{4\pi|\vec{r}|^2 w_{\vec{s}}} \tag{6}$$

Thus, the specific intensity of an electromagnetic wave emitted by a point source decreases with respect to the square of the traveled distance, which is in accordance to electromagnetic theory. However, this relation is always true, meaning that weights are basically free to choose.

$$I_{\nu,\vec{s}}(\vec{r}) \propto \frac{1}{|\vec{r}|^2} \tag{7}$$

In a next step, the scattering phase function $\Phi(\vec{s}', \vec{s})$ has to be discretized. The scattering phase function gives the angular distribution of scattered radiation and can be considered as a probability density function that determines the amount of radiation being scattered out of the solid angle $d\Omega_{\vec{s}'}$ into the solid angle $d\Omega_{\vec{s}}$. The shape of the function depends on the scattering regime (Rayleigh or Mie scattering) and can be estimated by the size parameter, which relates particle size to wavelength (Modest 2013). In case of microalgae biosuspensions, Mie scattering takes place and it was shown that the Henyey-Greenstein phase function Φ_{HG} is in good agreement with measured data of scattered light (Berberoglu et al. 2008, 2009). The main direction of scattering is defined by the asymmetry factor g, which is equal to the mean cosine of the phase function. The cosine of the scattering angle $cos(\theta)$ is defined by the two directions under consideration.

$$\Phi_{HG}\big(cos(\theta)\big) = \frac{1}{4\pi}\frac{1-g^2}{\big(1+g^2-2g\,cos(\theta)\big)^{3/2}} \tag{8}$$

The discretized phase function has to fulfill two conditions, namely conserving energy (zeroth moment equal to 1) and asymmetry (first moment equal to g). A common way to discretize the phase function in Discrete Ordinate Methods is to calculate discrete values from the scattering angles. However, in case of strong anisotropy ($|g| > 0.7$), this approach leads to a significant violation of energy conservation (in the order of 10^1 to 10^2) due to the overestimation of forward or backward scattering and causes the need of normalization to fulfill the conservation conditions (Hunter & Guo 2012). In this work, the phase function is discretized by carrying out the integral

$$\Phi_{HG\,\vec{s},\vec{s}'} = \frac{1}{4\pi w_{\vec{s}'}}\int\limits_{d\Omega_{\vec{s}'}}\frac{1}{4\pi w_{\vec{s}}}\int\limits_{d\Omega_{\vec{s}}}\Phi_{HG}\big(cos(\theta)\big)\,d\Omega_{\vec{s}'}\mathrm{d}\Omega_{\vec{s}} \tag{9}$$

numerically to calculate a representative mean, capturing scattering from all possible directions within the solid angle $d\Omega_{\vec{s}'}$ into all possible directions represented by the solid angle $d\Omega_{\vec{s}}$. Replacing the solid angles with the polar angles γ and the azimuth angles ϕ by using

$$d\Omega = \sin(\gamma)\,d\gamma d\phi \tag{10}$$

leads to a quadruple integral where the scattering angle is given by

$$\cos(\theta) = \sin(\gamma_{\vec{s}})\sin(\gamma_{\vec{s}'})\cos(\phi_{\vec{s}} - \phi_{\vec{s}'}) + \cos(\gamma_{\vec{s}})\cos(\gamma_{\vec{s}'}). \tag{11}$$

As it can be seen from Figure 2, the approach here applied ensures conservation of energy with a maximum error in the order of 10^{-1}. However, the applied equal-quadrature scheme leads to increasing inaccuracy if anisotropy increases and necessitates the normalization of the discrete values. For this purpose, a direction-dependent normalization technique intro-

duced by Wiscombe (1976) is applied. The discrete values of the scattering phase function $\Phi_{HG\,\vec{s},\vec{s}'}$ are normalized by

$$\Phi'_{HG\,\vec{s},\vec{s}'} = \Phi_{HG\,\vec{s},\vec{s}'}\,(1+\alpha+\alpha') \tag{12}$$

in such a way that α and α' are the solutions of the equation system

$$\sum_{M} \Phi_{HG\,\vec{s},\vec{s}'}\,(1+\alpha+\alpha') = 1 \qquad \vec{s} = 1 \ldots M. \tag{13}$$

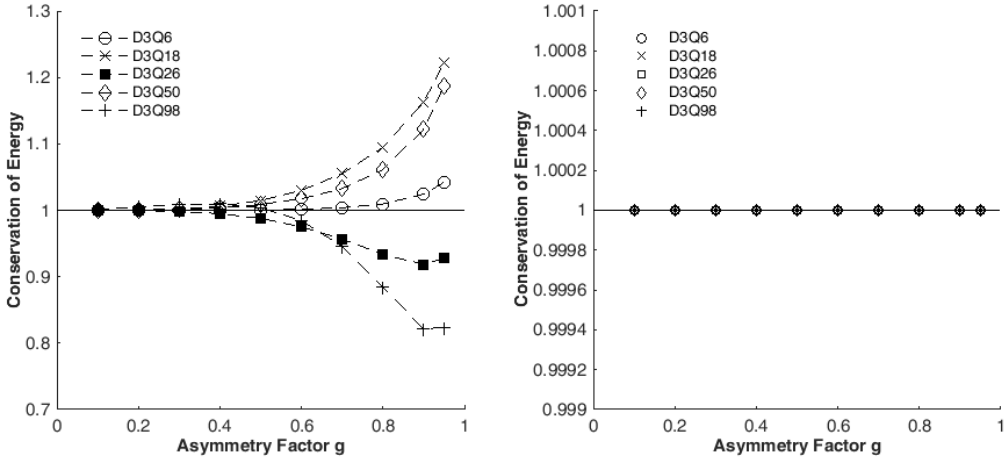

Figure 2: Conservation of energy, calculated as the numerical integral of Eq. (8) over the solid angle $d\boldsymbol{\Omega} = 4\boldsymbol{\pi}$. Left: before normalization; Right: after normalization.

In lattice Boltzmann methods, physical quantities are transferred into lattice units by means of non-dimensional quantities. For radiation transfer, the dimensionless optical depth τ is defined as follows.

$$\tau = \beta \Delta x \tag{14}$$

To ensure stability of the solution, the optical depth between two nodes in the lattice should stay below a threshold, which has to be specified in a grid convergence study. The number of nodes in one direction is then given by $N_x = \frac{L_0 \beta}{\tau} + 1$, where L_0 is the physical length of the simulation domain. By introducing the scattering albedo $\omega = \sigma/\beta$ and choosing $\Delta x_{LU} = 1$, the extinction, scattering and absorption coefficients can be transferred into lattice units.

$$\beta_{LU} = \frac{\beta \Delta x}{\Delta x_{LU}} \tag{15}$$

$$\sigma_{LU} = \omega \beta_{LU} \tag{16}$$

$$\kappa_{LU} = (1-\omega)\beta_{LU} \tag{17}$$

The fully discretized model equation is then given by

$$\begin{aligned} &I_{\nu,\vec{s}}(\vec{r} + c_{\vec{s}}\Delta t, t + \Delta t) - I_{\nu,\vec{s}}(\vec{r}, t) \\ &\qquad = \tau\, c_{\vec{s}} \frac{\Delta t_{LU}}{\Delta x_{LU}} \left(- I_{\nu,\vec{s}}(\vec{r}, t) + \omega \sum_{M} w_{\vec{s}'} I_{\nu,\vec{s}'}(\vec{r}, t)\, \Phi_{HG\,\vec{s},\vec{s}'} \right) \end{aligned} \tag{18}$$

and the mean specific intensity at every node can be calculated by

$$I_\nu(\vec{r}, t) = \sum_{\vec{s}} w_{\vec{s}}\, I_{\nu,\vec{s}}(\vec{r}, t). \tag{19}$$

Numerical Examples

In the following, the effects of spatial and angular discretization as well as the accuracy of the method shall be studied by comparison with Monte Carlo simulations as a reference. The lattice Boltzmann model was implemented in MATLAB R2014b. The algorithm follows the typical procedure in lattice Boltzmann simulations until a steady-state is reached. During the collision step, the right-hand side of Eq. (18) is calculated and added to the recent values $I_{\nu,\vec{s}}(\vec{r},t)$. Then, boundary conditions at walls and light sources are applied. Finally, the propagation of photons occurs in the streaming step. Steady-state is reached, if the condition

$$I_{\nu,\vec{s}}(\vec{r},t) - I_{\nu,\vec{s}}(\vec{r},t-\Delta t) \leq 10^{-6} \tag{20}$$

is true for any direction at any location on the lattice.

To study the effects of spatial and angular discretization, two examples are defined. In both cases, the domain is a cube with edge length of $1\ cm$, filled with an absorbing and scattering medium. The absorption and scattering coefficients were set to $0.5\ cm^{-1}$ each. In case 1, one surface emits radiation isotopically, while in case 2 a collimated beam with radius $r = 0.1\ cm$ enters the domain originating from the center of one surface. The boundary conditions at the light source were set to $I_{\nu,\vec{s}} = w_{\vec{s}} I_0$ in case 1 and in case 2 to $I_{\nu,\vec{s}} = 0$ for all directions except from the one normal to the surface, which was set to $I_{\nu,1} = I_0$. All walls are considered to be fully transparent and the boundary condition was set to $I_{\nu,\vec{s}} = 0$ for all directions. The same condition was applied to initialize the domain. The specific intensity was evaluated at the positions of nodes on the coarsest grid and discretization error was calculated according to Ferziger & Peric (2002).

As it can be seen from Figure 3, the solution converges and a stable solution can be reached by keeping the optical depth below $\tau \leq 0.025$. At the same time, increasing the angular resolution increases the accuracy of simulations in all cases. In particular, applying higher order velocity sets (D3Q50, D3Q98) increases the accuracy of simulations significantly.

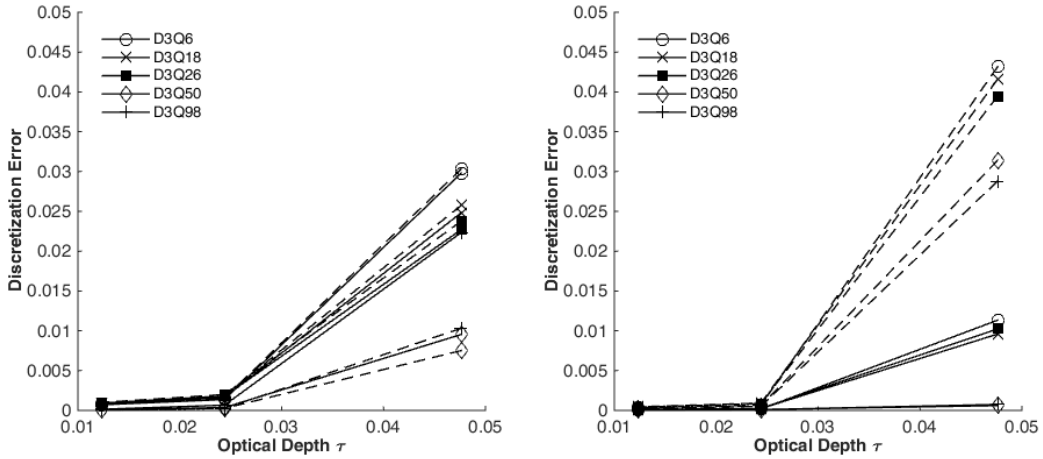

Figure 3: Discretization error with respect to optical depth and angular discretization. Solid lines indicate isotropic scattering, dashed lines indicate anisotropic scattering ($\boldsymbol{g} = \mathbf{0.9}$). Left: case 1; Right: case 2 (see text for details).

To study the accuracy of the method, the lattice Boltzmann prediction of case 2 is compared with Monte Carlo simulations. An open source Monte Carlo code for radiative transfer in biological tissue (Jaques et al. 2014) was used and medium properties were adapted to the given task. The Monte Carlo algorithm tracks photons along their path through the domain. At randomly chosen locations, the intensity of photons is evaluated and photons are scattered

according to the probability function as given by the integral of Eq. (8). If the intensity of a photon is below a threshold, it is not tracked anymore.
Optical depth was set to $\tau = 0.0244$ for the D3Q98 lattice Boltzmann method. For Monte Carlo simulations, 1.517E07 photons have been tracked and spatial discretization was set to 100 voxels in each dimension. Absorption and scattering coefficients were set as before, the asymmetry factor was chosen as $g = 0.9$. For comparability, intensity was normalized to irradiation per unit surface.
Figure 4 shows intensity profiles in the xy-plane at $z/Z_0 = 0$, which is half of the domain height. In the center of the collimated beam ($y/Y_0 = 0$), the prediction by the lattice Boltzmann method is in excellent agreement with Monte Carlo simulations. In regions illuminated only by scattered radiation, both methods provide similar results until a certain point where deviations suddenly increase. This is also confirmed by intensity profiles with respect to domain width, as shown in Figure 4. While at $x/X_0 = 0.1$ both methods are in good agreement, far off the light source the lattice Boltzmann method deviates from Monte Carlo simulations.

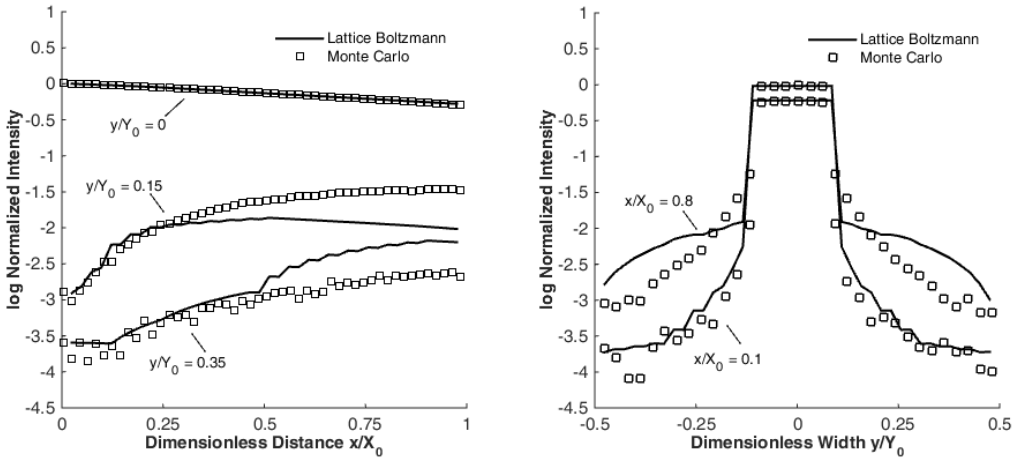

Figure 4: Profiles of specific intensity predicted by lattice Boltzmann method and Monte Carlo method on the xy-plane at $z/Z_0 = 0$. The center of the collimated beam located at $y/Y_0 = 0$. Left: intensity with respect to traveled distance; Right: intensity with respect to domain width.

A likely explanation for deviations between both methods is the Ray effect, which is a well-known problem in Discrete Ordinate Methods (Chai et al. 1993). Ray effect is caused by the angular discretization of continuous waves and is usually addressed by increasing the angular resolution. Figure 5 shows a contour plot of the specific intensity field as predicted by lattice Boltzmann method and Monte Carlo method, respectively. As already indicated, near the light source both methods are in good agreement, while with increasing distance to the light source the gradients of intensity adhere to discrete directions in the lattice Boltzmann simulation. However, regardless of this inaccuracy, the lattice Boltzmann method can be applied to accurately predict the attenuation of a collimated beam in a microalgae biosuspension.

Attenuation of Light Intensity in a Microalgae Biosuspension

To experimentally validate the lattice Boltzmann model, the microalgae *Chlamydomonas reinhardtii* cc125 was cultivated in Basal Medium with soil extract under continuous illumination in Erlenmeyer flasks. After six days of cultivation, light attenuation in different dilutions of the biosuspension (1:5, 1:10, 1:20) was spectrophotometrically determined. Cell concentration of the undiluted culture was examined in 8-fold determination in a hemocytometer at $5.464\ 1E06\ ml^{-1}$ and 95 % confidence interval of $\pm 0.754\ 1E06\ ml^{-1}$. Pigment content of

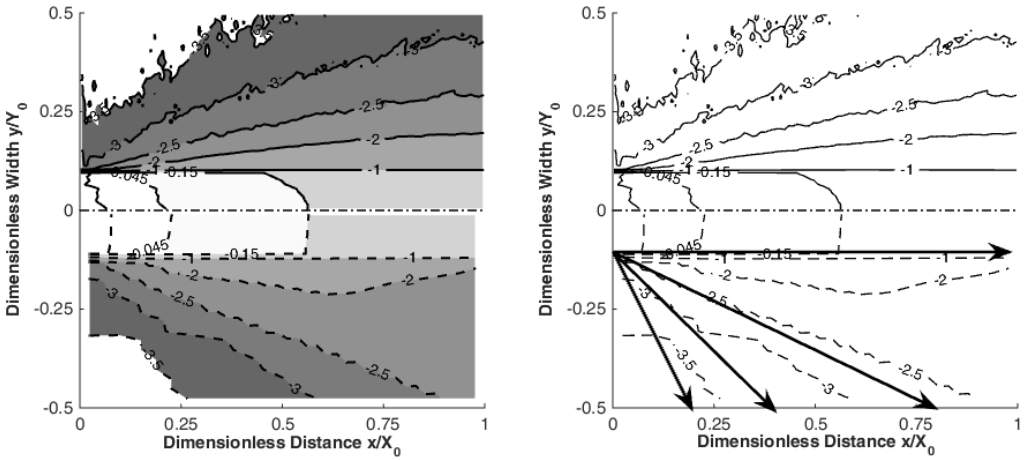

Figure 5: Contour plot of predicted specific intensity on the xy-plane at $z/Z_0 = 0$. Contour levels denote log Normalized Intensity. Top: prediction by Monte Carlo method; Bottom: prediction by lattice Boltzmann method. In the right plot, discrete directions in lattice Boltzmann are indicated by arrows.

Chlorophyll *a* and *b* was determined according to Porra et al. (1989) and was used to calculate the spectral absorption index of algae cells k, which is related to the imaginary part of the complex index of refraction by the relation $n'' = k\lambda/4\pi$. From literature, the real part of the complex index of refraction $n' = 1.36$ (Lee et al. 2013) and the asymmetry factor $g = 0.96$ (Dauchet et al. 2015) were taken and assumed to be constant across the whole spectrum in a first approximation. The equivalent diameter of the spherical cells according to Dauchet et al. (2015) was calculated from flow particle imaging (Sysmec FPIA3000) and set to $8.465\ \mu m$. The refractive index of the growth medium was measured at $n_m = 1.333$. Finally, the absorption and scattering coefficients were calculated by using the Anomalous Diffraction Approximation (van de Hulst 1957).

Figure 6 compares the predicted attenuation of light with experimental measurements. It can be seen that the results are in good agreement for both wavelengths considered. The maximum absolute and relative errors are 0.0152 and 0.0164, respectively. To further increase the accuracy of simulations, optical properties of the biosuspension have to be precisely calculated from cell composition. This applies particularly to the real part of the complex index of refraction of microalgae cells, since the attenuation of the collimated beam is basically caused by out-scattering and the prediction of the radiative field in the whole domain will be highly affected by the careful selection of optical properties.

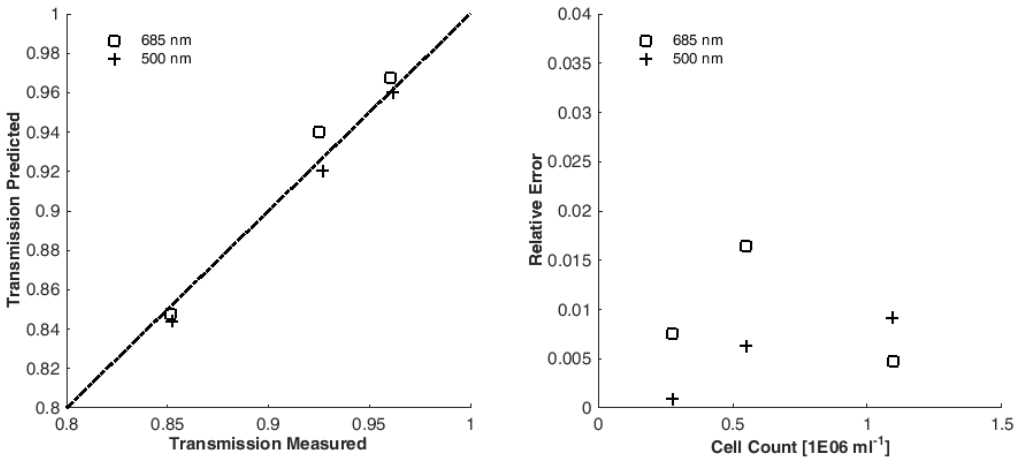

Figure 6: Comparison between predicted attenuation by the lattice Boltzmann method and experimental measurements at different wavelengths. Left: absolute transmission; Right: relative error.

Conclusions

In this paper, a lattice Boltzmann framework to predict radiative transport in biosuspensions was presented. To the best knowledge of the authors, this is the first application of a lattice Boltzmann framework for the simulation of radiative transport in three dimensions. The predicted fields of specific intensity were basically in good agreement with Monte Carlo simulations. However, significant deviations between both methods can be noticed in regions illuminated only by scattered light. Basically, there are two possible reasons, both associated with the solution of the discretized scattering integral. The first potential cause is due to the Ray effect and an increase of accuracy could be possibly reached by the development of a correction term, which could be easily implemented into the lattice Boltzmann framework similar to in-scattering. A second potential cause of inaccuracy is the chosen quadrature scheme, which affects the discretization of the scattering phase function. By developing more accurate quadrature schemes, a precise calculation of discrete values will increase the accuracy of the lattice Boltzmann method. To detect the main cause of inaccuracy and weaknesses of the method, more test cases have to be validated, both numerically and experimentally. However, the prediction of light attenuation in a microalgae biosuspension by the lattice Boltzmann method was already in good agreement to experimental measurements, with the restriction that the experimental evaluation of the full intensity field is still pending. In biosuspensions, it must be taken into account that the optical properties of cells are subject to uncertainty and moreover, may change dynamically during cultivation. For optimization of cultivation plants, this means that it is not sufficient to accurately predict radiative transfer alone. Moreover, the usage of dynamic models of algae metabolism, the prediction of radiative properties from cell properties as well as the coupling to flow solvers is required. Due to their flexibility, lattice Boltzmann methods appear to be a promising tool to successfully solve this optimization task.

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