Applied Mathematics and Computation 319 (2018) 59–70

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Spectral simulation of light propagation in participating media by using a lattice Boltzmann method for photons

Christopher McHardy*, Tobias Horneber, Cornelia Rauh

Chair of Food Biotechnology and Food Process Engineering, Technische Universität Berlin, Berlin, Germany

ARTICLE INFO

Article history:
Available online 9 February 2017

Keywords:
Radiation transfer
Lattice Boltzmann method
Spectral simulation
Adaptive quadrature
Photobioreactor
Microalgae

ABSTRACT

A lattice Boltzmann method for radiation transfer and Newton–Cotes formulas are used in this work to compute the propagation of polychromatic light in a biosuspension of phototrophic microorganisms. The polychromatic light field is obtained from monochromatic lattice Boltzmann simulations by integration across the visible spectrum. The effects of the spectral resolution, radiation characteristics and the chosen integration rule on the accuracy of the integration are investigated. It was found that reasonable results can be achieved on equidistant spectral grids with a grid spacing of $\Delta\lambda \leq 20\,\text{nm}$, although error compensation might be a serious issue if the trapezoidal rule is applied. Based on *a priori* information about the light field, an approach for the computation of adapted spectral grids is introduced, which aims at the efficient computation of polychromatic light fields. It was found that no significant increase of accuracy can be realized by usage of adapted spectral grids for spectral integration. It is presumed that this observation is caused by the changing shape of the light spectrum along the optical path.

1. Introduction

In recent times, the cultivation of phototrophic microorganisms in photobioreactors receives increasing attention from science and industry. This interest is caused by the ability of such organisms to drive their metabolism by solar energy, and, at the same time, to accumulate huge amounts of various metabolites, making phototrophic microorganisms to be considered as a sustainable feedstock for the production of biomass, biofuels, food, feed and pharmaceuticals [1,2]. However, taking advantage of these beneficial characteristics is still limited by high costs for cultivation and processing of biomass. In particular, mixing becomes a matter of expense due to the necessity of moving cells between light and dark zones in photobioreactors since the availability of light in photobioreactors is known to be a key factor for growth and productivity [3]. Due to this importance, accurate predictions of the spatial light distribution become indispensable for design and optimization of photobioreactors and control of biomass production.

Light propagation in participating media is governed by the radiation transfer equation (RTE). Numerical solutions of the RTE can be obtained by different methods, such as Monte Carlo methods (MCM), Discrete Ordinate methods (DOM) or Finite Volume methods (FVM). All of these methods are well documented and further information can be found elsewhere [4,5]. A new class of methods to solve the RTE are lattice Boltzmann methods (LBM). The idea of using a lattice Boltzmann approach seems to be straightforward since the RTE can be interpreted as a Boltzmann-type transport equation for photons. Moreover,

* Corresponding author.
E-mail address: christopher.mchardy@tu-berlin.de (C. McHardy).

http://dx.doi.org/10.1016/j.amc.2017.01.045

in addition to radiative transfer, many engineering applications also require the consideration of flows so that a consistent methodology to solve multiphysical problems seems to be beneficial. Enormous improvements have been achieved in the development of LBM for various hydrodynamic tasks [6–10], making the LBM a potential candidate for providing a powerful multiphysical simulation framework.

Originating from works of Asinari et al. [11], Ma et al. [12] and Bindra and Patil [13], a number of further developments have been made in the last years, basically dealing with radiation transfer in 1D and 2D geometries [14–18], while radiation transfer in 3D was rarely considered [19–21]. As a remarkable development, recently, the linkage of the mesoscopic lattice Boltzmann Bhatnagar–Gross–Krook (LBGK) equation and a macroscopic target equation for radiation transfer by means of Chapman–Enskog expansion was demonstrated [19,20]. This approach differs from other models in the sense that usually the target equation was the mesoscopic RTE itself [13,21], which is also true for other numerical methods, such as the DOM or the FVM. However, approximating a macroscopic target equation by solving a lattice Boltzmann equation is what is usually done in fluid dynamics, where the LBM has its origin [6].

All of the above mentioned models have in common that monochromatic radiation transfer is solved. However, radiation characteristics of participating media as well as the spectrum of radiation sources are most often characterized by wavelength-dependency. This is also relevant for photobioreactors, where spectral absorption and scattering characteristics of the microorganisms have to be taken into account and different types of light sources (sunlight, artificial sources) might be used for illumination [22–24]. Spectral-dependent radiation properties require the computation of monochromatic radiation fields and the subsequent superposition of solutions to gain polychromatic profiles of light intensity. Obviously, the accompanied increase of computational costs depends on the desired degree of spectral resolution, becoming maximum for resolving every single wavelength in the visible spectrum. A common approach to deal with polychromatic radiation transfer is to distribute a finite number of discretization points over the spectrum and compute monochromatic radiation fields at the chosen wavelengths. Afterward, the monochromatic field quantities are integrated across the spectrum by means of numerical integration rules (*e.g.*, Newton–Cotes rules) to gain the polychromatic light field. In the field of photobioreactor research, this approach as well as the comparable WSGG model (Weighted Sum of Gray Gases) have been applied with different degree of spectral resolution [25–27]. However, despite of its significant importance, the questions of minimizing the number of discretization points and their optimal placement in the spectral grid remains unanswered in the literature.

The present contribution aims at closing this gap. Effects of spectral discretization and numerical integration rules on the accuracy of polychromatic intensity profiles are investigated. Therefore, numerical solutions of the RTE are computed by means of a lattice Boltzmann method, incorporating three-dimensional scattering. Typical radiation characteristics of microalgae as well as a geometry similar to flat-panel photobioreactors and light sources which are relevant for cultivation of microalgae are assumed. In addition, an approach for the optimal placement of discretization points in the spectral grid is developed and tested. The paper is organized as follows: in Section 2, the choice of the lattice Boltzmann model is motivated by considering typical radiation characteristics of microalgae. Also the model equations and numerical quadrature rules are introduced. In Section 3, details concerning the simulation setup are specified. Results for monochromatic and polychromatic light fields are presented in Section 4, followed by the presentation and evaluation of non-uniform spectral grids for the calculation of polychromatic light fields. Finally, a discussion of the results and conclusions are given in Section 5.

2. Computational methods

2.1. Radiation transfer equation

The radiation transfer equation reads,

$$\frac{1}{c}\frac{\delta J}{\delta t} + \mathbf{n}\nabla_{\mathbf{x}} J = -\beta J + \kappa J_e + \frac{\sigma}{4\pi}\int_{4\pi} J'\Phi(\mathbf{n}', \mathbf{n})\mathrm{d}\Omega'. \tag{1}$$

Herein, J denotes the intensity of radiation, characterizing the amount of photons which propagate into direction $\mathbf{n}$ and solid angle $\mathbf{\Omega}$ with speed of light c. The extinction coefficient $\beta = \kappa + \sigma$ measures the interaction of photons with matter due to absorption and scattering, both individually expressed by absorption (κ) and scattering (σ) coefficients. Scattering re-distributes photons from directions $\mathbf{n'}$ into the direction of propagation $\mathbf{n}$ according to an angular probability density function $\Phi(g, \mathbf{n}, \mathbf{n'})$, known as the scattering phase function, where the asymmetry factor g is the cosine of the mean scattering angle. Because of its low relevance for photobioreactors, the re-emission of absorbed photons by fluorescence with intensity J_e is neglected from now on.

2.2. Lattice Boltzmann method for photons

2.2.1. Selection of the lattice Boltzmann model

In Section 1, it was mentioned that recently the linkage of the LBGK equation to a macroscopic target equation was demonstrated by [18–20]. This linkage is very beneficial from a computational point of view since it ensures convergence rates of second order in space and time. In contrast, as pointed out by Yi et al. [18], prior models are consistently characterized by first order convergence rates. However, deviating from fluid dynamics where the Navier–Stokes equations govern the fluid motion on macroscopic scales, in radiation transfer modeling the mesoscopic RTE is commonly considered as the