Journal of Quantitative Spectroscopy & Radiative Transfer 128 (2013) 52–59

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

The practice of recent radiative transfer Monte Carlo advances and its contribution to the field of microorganisms cultivation in photobioreactors

Jérémi Dauchet [a,c,d,*], Stéphane Blanco [c,d], Jean-François Cornet [b], Mouna El Hafi [e], Vincent Eymet [e], Richard Fournier [c,d]

[a] Clermont Université, Université Blaise Pascal, Institut Pascal - UMR 6602, BP 10448, F-63000 Clermont-Ferrand, France
[b] Clermont Université, ENSCCF, Institut Pascal - UMR 6602, BP 10448, F-63000 Clermont-Ferrand, France
[c] Université de Toulouse; UPS, INPT; LAPLACE (Laboratoire Plasma et Conversion d'Energie); 118 route de Narbonne, F-31062 Toulouse cedex 9, France
[d] CNRS; LAPLACE; F-31062 Toulouse, France
[e] Université de Toulouse; Mines Albi; CNRS; Centre RAPSODEE, Campus Jarlard, F-81013 Albi cedex 09, France

ARTICLE INFO

Article history:
Received 26 June 2012
Accepted 9 July 2012
Available online 16 July 2012

Keywords:
Radiative transfer
Monte Carlo
Multiple scattering
Zero-variance
Photobioreactor
Microalgae

ABSTRACT

The present text illustrates the practice of integral formulation, zero-variance approaches and sensitivity evaluations in the field of radiative transfer Monte Carlo simulation, as well as the practical implementation of the corresponding algorithms, for such realistic systems as photobioreactors involving spectral integration, multiple scattering and complex geometries. We try to argue that even in such non-academic contexts, strong benefits can be expected from the effort of translating the considered Monte Carlo algorithm into a rigorously equivalent integral formulation. Modifying the initial algorithm to simultaneously compute sensitivities is then straightforward (except for domain deformation sensitivities) and the question of enhancing convergence is turned into that of modeling a set of well identified physical quantities.

1. Introduction

During the last 15 years, significant methodological advances have been reported in the field of Monte Carlo simulation of linear transport phenomena, in particular as far as radiative transfer is concerned [1–3]. Among them, attention is here devoted to integral formulation, zero-variance approaches [4,5] and sensitivity evaluations [6], as well as to the question of implementing practically the corresponding algorithms when thinking of realistic systems involving spectral integration, multiple scattering and complex geometries. Such techniques all rely on the premise that Monte Carlo algorithms can be designed in more subtle ways than making direct analogies with the statistics of corpuscular transport. But along this line a main advantage of Monte Carlo practice seems to be lost. The fact that standard radiative transfer Monte Carlo codes can be pictured as close translations of well established physical pictures of photon emission, diffusion, scattering, reflection and absorption implies indeed that such codes are easy to design and easy to upgrade toward the representation of additional (or further accurate) physical phenomena. If the use of advanced Monte Carlo techniques implies that these physical pictures are hidden behind complex algorithmic tricks, or that the corresponding codes become so complex that implementation and upgrading are sources of strong practical

---

[*] Corresponding author at: Clermont Université, Université Blaise Pascal, Institut Pascal - UMR 6602, BP 10448, F-63000 Clermont-Ferrand, France. Tel.: +33 (0)4 73405317.
E-mail address: jeremi.dauchet@laplace.univ-tlse.fr (J. Dauchet).

0022-4073/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jqsrt.2012.07.004

difficulties, then radiative transfer specialists will be reluctant to make an effective use of these techniques, whatever their expected benefits. We try to argue here (and illustrate with a photobioreactor example) that these drawbacks vanish as soon as a strict relationship is made, in an explicit manner, between the considered linear transport Monte Carlo algorithm and the corresponding integral transport formulation. Provided that the relationship is made systematically, whatever the complexity of the problem, the whole reasoning can be made in terms of radiative transfer formulations, keeping all the immediate benefits of available physical pictures. This also implies that the technical aspects that have no direct relation with physical reasoning, in particular the statistical treatments, parallelization, pure geometrical considerations, etc, can all be translated into scientific computation libraries and can be used in quite straightforward manners.

Photobioreactors are processes of biomass production in which photosynthesis is catalyzed by photosynthetic microorganisms in aqueous suspensions constituting non-gray absorbing and anisotropically scattering media. Careful radiation transfer analysis of photobioreactors is identified as the clue for efficient design and efficient operation [7–11]. Monte Carlo methods seem to be appropriate for such an analysis since they allow to tackle the intermediate optical depths and quite complex geometries that are encountered in this context. The present work focuses on a cylindrical reactor prototype (cultivating the micro-algae *Chlamydomonas reinhardtii*) in which the incident solar light flux density is diluted in the volume of culture thanks to a thousand of light-diffusing optical fibers emitting a quasi homogeneous density flux on the totality of their surface. All details and the corresponding notations are provided in Figs. 1 and 2 (the microorganism density η is uniform within the culture volume $\mathcal{V}$, emission is negligible, $k_{a,\nu}=\eta\sigma_{a,\nu}$ and $k_{s,\nu}=\eta\sigma_{s,\nu}$ are the absorption and scattering coefficients). The following methodological discussions address the estimation of the specific number of photons $A(\mathbf{x}_0)$ absorbed in the photosynthetically active radiation domain $[\nu_{min},\nu_{max}]$, at a location $\mathbf{x}_0$ within the microorganism suspension:

$$\begin{aligned} A(\mathbf{x}_0) &= \frac{1}{\eta}\int_{\nu_{min}}^{\nu_{max}} d\nu \int_{4\pi} d\boldsymbol{\omega}_0 k_{a,\nu}\frac{L_\nu(\mathbf{x}_0,-\boldsymbol{\omega}_0)}{h\nu} \\ &= \int_{\nu_{min}}^{\nu_{max}} d\nu \int_{4\pi} d\boldsymbol{\omega}_0 \sigma_{a,\nu}\frac{L_\nu(\mathbf{x}_0,-\boldsymbol{\omega}_0)}{h\nu} \end{aligned} \qquad (1)$$

where $L_\nu(\mathbf{x}_0,-\boldsymbol{\omega}_0)$ is the intensity at $\mathbf{x}_0$ in the direction $-\boldsymbol{\omega}_0$ at frequency ν, and h is Planck's constant. $A(\mathbf{x}_0)$ locally determines the kinetics of production within the culture volume since it represents the energy that enters the photosynthesis [7]. The surface productivity of photobioreactors is directly linked to their energetic efficiency which estimation implies to calculate $A(\mathbf{x}_0)$ for more than 10^6 different locations in order to evaluate the production rates integrated over the whole reactor volume (which cannot be done inside the presented Monte Carlo algorithm since the local production rates are non-linear functions of $A(\mathbf{x}_0)$). This calculation is then repeated for several sets of operational and design parameters, as a part of design/operation optimization procedures. Therefore, the reduction of the calculation times and the opportunity to estimate sensitivities of $A(\mathbf{x}_0)$ at low calculation costs (in order to accelerate the optimization procedures, thinking for example of a method of steepest descent) both constitute important practical concerns. For these reasons, the simulations presented hereafter are parallelized and make use of computation tools developed by the computer graphics research community for the acceleration of photon tracking in complex

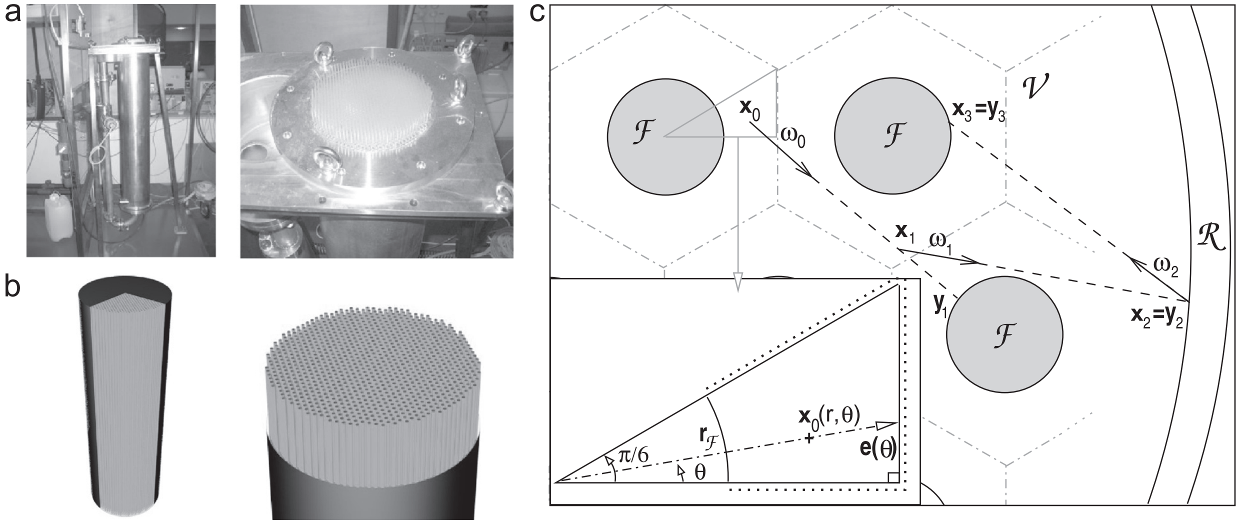

Fig. 1. (a) Prototype of solar volumetrically lightened photobioreactor [8]. (b) EDStar geometry: both the reactor ($\mathcal{R}$) and the 979 light-diffusing optical fibers ($\mathcal{F}$) are cylinders of height 1 m; reactor diameter is 16.5 cm; distance between two fiber axis is $d_{\mathcal{F}}=4.8$ mm; fiber radius is $r_{\mathcal{F}}=1.2$ mm. $\mathcal{R}$ and $\mathcal{F}$ are diffuse-reflective with uniform reflectivities $\rho^{\mathcal{R}}$ and $\rho^{\mathcal{F}}$ respectively. $\mathcal{F}$ is Lambertian emitting with a uniform surface flux density φ_ν. (c) 2d hexagonal lattice fiber arrangement; an optical path example within the culture medium $\mathcal{V}$; at the bottom left, description of how the location of $\mathbf{x}_0$ is defined around a given fiber ($e(\theta)=(d_{\mathcal{F}}/2)1/\cos(\theta)$).