Numerical simulations of fluid flow and light distribution inside bio-reactors
Nummerische Simulation von Stroemung und Lichtverteilung in einem Bioreaktor

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Abstract

The design of bio-reactors for the cultivation of algae suffers from inadequate scale up of technical parameters from laboratory to large scale. Numerical simulations of processes are generally performed without taking into account the presence of algae. Furthermore, lack of information about fluid-mechanic quantities which influence the growth and the concentration of algae is found in literature. We numerically simulate the bubble column flow in a cylindrical bio-reactor considering continuous and dispersed phases, i.e. water and air. In order to simulate the presence of algae, we inject and track small particles of size of the order of microns from four different positions inside the reactor. By means of an open source Monte Carlo code, we study the light distribution affected by the presence of algae inside in a 1 mm^3 volume at a certain time step. Numerical results reveal shadowed zones due to the presence of particles, which may strongly affect the growth of algae.

Introduction

Bubble column reactors are commonly utilized in biotechnological industries, since they are easy to construct and to operate with (Lobaton et al. 2011). Besides, they require low maintenance. An accurate prediction of the flow field inside bioreactors is crucial to determine the level of shear stress on algal cells, as well as light/dark cycles. Shear stresses which generates during bubble coalescence and break-up, and eddies whose length scale is comparable to cell sizes may damage algal cells (Eleftherios et al.1993). On the other hand, light/dark cycles are decisive for the photosynthesis.

Quantitative information of fluid flow can be obtained experimentally, for instance with laser Doppler anemometry (LDA) (Julia et al. 2007), computer-automated radioactive particle tracking (CARPT) (Sanyal et al. 1999), or computer tomography (CT) (Dhotre et al. 2004). However, they are expensive and sometimes be difficult to implement. On the other hand, numerical simulations are less costly and provide detailed information of the flow field.
Two dimensional transient simulations of fluid flow date back to more than a decade ago. They have always been a useful tool in terms of model development, and allowed for testing of several turbulence models, i.e. k - ε , k - ω and the turbulence mixing length (Bech et al. 2005). However, they are sensible to grid refinement and may produce non-physical results.
Only three dimensional unsteady simulations are able to successfully capture the complex characteristics of bubble column flows. Former numerical simulations were performed mainly focusing on turbulence modeling of continuous and dispersed phases (Pfleger et al. 2001). Recently, the contribution of the so-called non drag forces, i.e. lift, virtual mass, wall lubrication and turbulent dispersion forces has been added. It has been recognized that they strongly influence the time averaged liquid and gas velocity profiles (Masood et al. 2014).
Additionally, inclusion of internals have been considered. It has been found that the inclusion of plates increases the gas holdup by 79% and the mixing time by 48% (Lobaton et al. 2011).
On the other hand, the distribution of light in bioreactors is one of the most important factors affecting the growth of microalgae, since local light intensities are used as input for biological models that predict growth and reactor performance (Bechet 2013).
A detailed review of light transfer in algal cells, as well as issues related to cultivation of micro-algae in bio-reactors can be found in (Wang et al. 2014). It contains an exhaustive description of how algal cells interact with light, considering also the light attenuation as soon as it enters a photo-bioreactor (PBR). Besides, this review focusses on characteristics of algae cultivation, i.e., light source, wavelength, intensity, effects of light/dark cycles and flashing light effects. In the end, strategies to improve the light utilization efficiency are also suggested.
Integrated models consisting of CFD, light distribution and growth kinetics of algae cells are present in literature. For instance, CFD simulations have been combined with Lambert Beer law and Aiba model (Zhang et al. 2015), or with a compartmental modelling approach and photosynthetic factory model (Nahua et al. 2013).
In this work, we propose a combination between CFD and light distribution simulations. First we simulate the bubble column flow in a cylindrical bioreactor, and later we inject particles that simulate the presence of algae. We extract the position of particles inside a small volume at a specific time step, and then we numerically compute how light is distributed inside it. Shadowed zones results, altering the amount of light each particle receive.

Simulation set-up: CFD

Geometry and grid generation

The geometry is a cylindrical reactor with a small inlet: the length of the cylinder is 50 [cm] and its diameter is 9.4 [cm]. The diameter of the inlet is 4 [mm].
Due to its simplicity, both the geometry and the grid have been created by the commercial software ANSYS ICEM®. A structured mesh has been obtained by using two O grids, see Fig. 1. At present, we consider a coarse mesh equally spaced in the axial direction, which has 27234 elements.

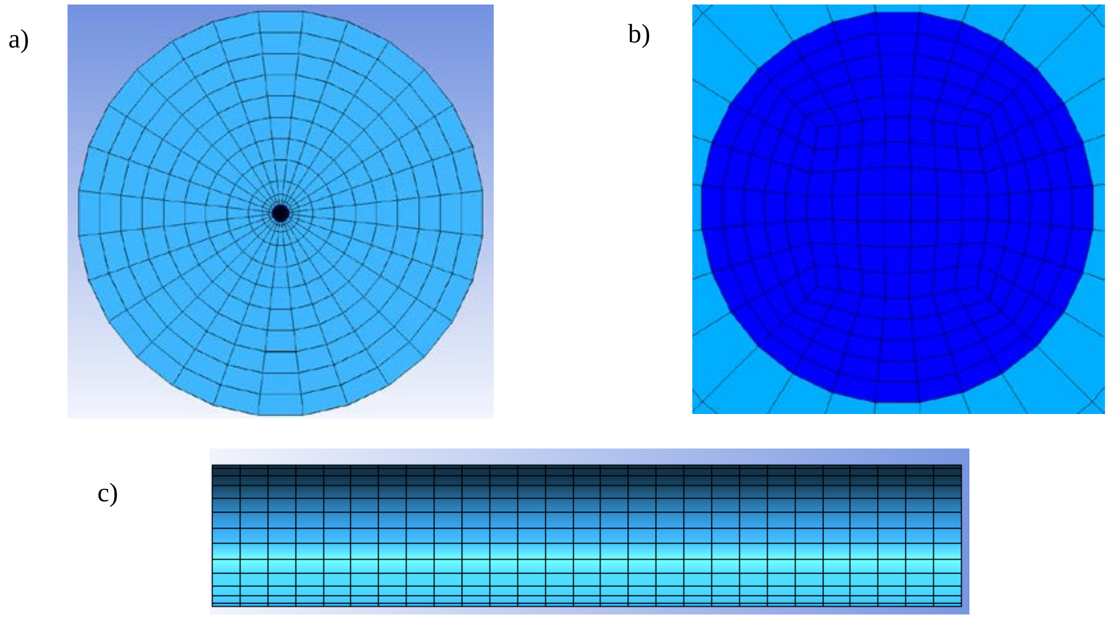

Fig. 1 a) meshed face of the cylinder containing the inlet, b) detailed view of the meshed inlet, c) lateral view: the final mesh has 27234 elements.

Mathematical modelling of fluid flow

We consider a full Eulerian-Eulerian approach for both dispersed and continuous phase. The mass conservation equations, one for each of the two phases, read

$$\frac{\partial}{\partial t}(\rho_k \alpha_k) + \nabla \cdot (\rho_k \alpha_k \boldsymbol{u}_k) = 0 \tag{1}$$

The index k indicates the phase, i.e. L for liquid, G for gas, ρ_k, α_k and $\boldsymbol{u}_k$ are the density, volume fraction and velocity of each phase k. In turn, the momentum equation assumes the form:

$$\frac{\partial}{\partial t}(\rho_k \alpha_k \boldsymbol{u}_k) + \nabla \cdot (\rho_k \alpha_k \boldsymbol{u}_k \boldsymbol{u}_k) = \nabla \cdot (\alpha_k \boldsymbol{\tau}_k) - \alpha_k \nabla p + \rho_k \alpha_k \boldsymbol{g} + \boldsymbol{M}_k \tag{2}$$

The terms on the left-hand side are the temporal and the convective acceleration, while those on the right-hand side are the turbulent stress tensor, pressure gradient, gravity and interphase momentum forces (Masood et al. 2014). The stress tensor reads

$$\boldsymbol{\tau}_k = \mu_{k,eff} \left[\nabla \boldsymbol{u}_k + (\nabla \boldsymbol{u}_k)^T \right] \tag{3}$$

where the fluid flow for both phases is considered incompressible. The effective viscosity $\mu_{k,eff}$ is the sum of two terms, that is, the molecular viscosity, and the turbulent one

$$\mu_{k,eff} = \mu_{k,Lam} + \mu_{k,Turb} \tag{4}$$

The so called "non-drag forces" term, $\boldsymbol{M}_k$, comprises the lift, virtual mass, wall lubrication and dispersion forces (Masood et al. 2014).
As soon as we inject particles, their position is tracked every time-step. The particle displacement is determined by the numerical integration of the following equation

$$\frac{d\boldsymbol{x}_P}{dt} = \boldsymbol{U}_P \tag{5}$$

and the particle velocity $\boldsymbol{U}_P$ is calculated by solving

$$m_P \frac{d\boldsymbol{U}_P}{dt} = \boldsymbol{F}_{all} \tag{6}$$

where $\boldsymbol{F}_{all}$ is the sum of the forces acting on a particle. Equation (5) and (6) are solved by means of a first order explicit Euler (ANSYS-CFX Solver Theory Guide 2013).

Simulation details

We numerically solve the system of equations (1)-(4) by the commercial software ANSYS CFX®, which is a finite volume solver. At the inlet, an air mass flow rate equal to 9.85*10^$^{-6}$ [kg/s] has been specified, while the outlet has been set as an opening. Additionally, an air headspace in the last 10 [cm] of the reactor has been left. The remaining parts of the geometry have been set as walls, and a free slip condition for the air and a no slip condition for the water have been imposed. Further, the mean bubble diameter has been set to 1 [cm]. The turbulence model adopted to calculate $\mu_{k,Turb}$ for the air phase is the dispersed phase zero equation, while the one chosen for the water is the Shear Stress Transport (SSH) one (ANSYS-CFX Solver Theory Guide 2013). The Grace correlation has been found suitable for computing the drag acting on bubbles, and the Legendre-Magnaudet formulation has been selected for the shear induced lift force acting on the disperse phase. The coefficient of the virtual mass forces has been fixed to 0.5. Besides, the wall lubrication forces have been defined using the Frank model and the turbulent dispersion forces have been considered with the aid of the averaged Favre model. The dispersion coefficient has been imposed equal to 1.
Unsteady simulations have been run up to 120 [s], and a time step of $5 \cdot 10^{-4}$ [s] ensured that the residuals of velocity, pressure and mass conservation converged below the value of 10^{-4}. After 100 [s], particles have been injected inside the reactor at particle rate of 20 [particles/s] from four different positions, in order to simulate the motion of algae. Four particles injection point cones have been selected: the first one at x=3 [cm], y=0 [cm], z=0.5 [cm], the second one at x=-3 [cm], y=8 [cm], z=0 [cm], the third one at x=3 [cm], y=20 [cm], z=0 [cm], and finally the fourth one at x=-3 [cm], y=29 [cm], z=0 [cm].
The one-way coupling method allows the particles to be transported by the flow without interfering with it, which is in accordance to the case of low particle Stokes number, St << 1. Besides, particles are only linked to one phase, i.e. the fluid, so there are no possibilities to find them in the dispersed phase. The maximum diameter of the particles is 10 µm and the minimum one is 1 µm with an average of 5 µm.

Simulation set-up: Light distribution

Theoretical background of Monte Carlo (MC) method

The principle behind the MC method is the tracing of single photons through the domain. Photons are launched at a source and propagate freely until they change their direction of propagation due to scattering by matter. The new direction of propagation after a scattering event is sampled from a probability density function, i.e. the scattering phase function.
The domain is discretized in to125000 cubic voxels in which the recent energy of a photon is stored if it passes through a voxel. Due to cells absorption, the energy a photon carries may be lowered on its path through the domain. The tracing stops if a photon leaves the domain

through the open boundaries, or its energy falls below a threshold. A detailed description of the Monte Carlo algorithm is given by Wang et al. (1995).
Local scattering and absorption depend on scattering and absorption coefficients σ and κ which must be assigned to each voxel. The scattering and absorption coefficients in a volume are related to the scattering and absorption cross-sections a_{sca} and a_{abs} of individual cells. In case of diluted suspensions, the relation is linear, i.e.

$$\sigma = a_{sca} c$$

$$\kappa = a_{abs} c$$

where c denotes the concentration of the cells per volume, which is the volume of a voxel in the present case. The scattering and absorption cross-sections of individual cells were computed by means of the Anomalous Diffraction Approximation (van de Hulst 1957).
A complex index of refraction of microalgae cells of $n = 1.352 + i0.0042$ has been assumed at wavelength $\lambda = 680$ [nm], which corresponds to the absorption maxima of pigments in microalgae cells (Lee et al. 2013). Mie-Scattering of microalgae has been approximated by the Henyey-Greenstein phase function with an anisotropy factor $g = 0.98$ (Dauchet et al. 2015). The Monte Carlo simulations have been performed by using an Open Source solver (Jaques et al. 2014).

Results and discussion

A typical characteristic of an aerated bioreactor flow is a meandering air bubble "plume". Considerations of a single bubble rising in a denser liquid provide useful insights into the more complex phenomenon of an oscillating bubble column.

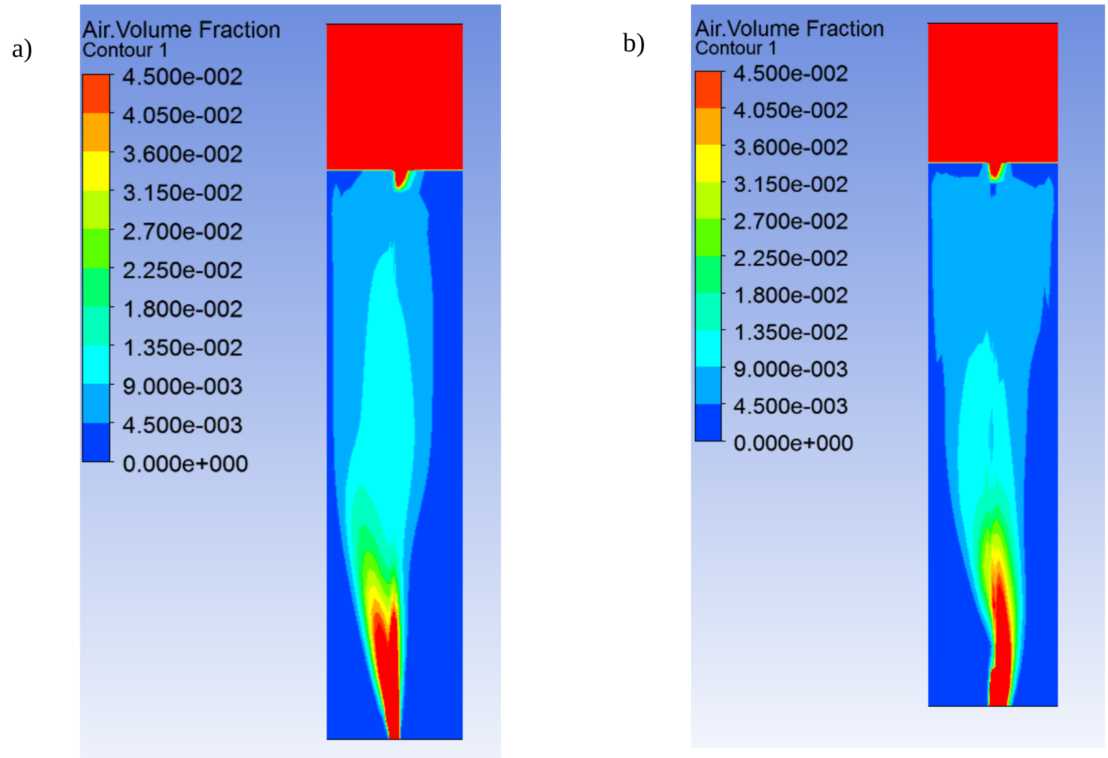

Fig. 2 a) Air Volume Fraction on an x-y plane at z=0 at t=47.6 [s], b) Air Volume Fraction on an x-y plane at z=0 at t=57.6 [s]. The mass flow rate is 9.85*10^-6 [kg/s]

A bubble rises in a quiescent liquid due to the buoyancy force that induces an upward motion, and it continuously accelerates as long as the buoyancy force is greater than the drag force. The acceleration causes a pressure gradient between the top and the bottom surface of a bubble that produces a liquid jet, responsible for the deformation of the shape of a bubble (Hua et al. 2007). Besides, as the bubble rises, velocity increases and an asymmetric wake generates behind the bubble, which provokes its zigzag movement.
The plume oscillation is clearly reproduced in the simulations. For instance, results concerning a contour of air-volume fraction in a cross-sectional (x-y) plane are presented in Fig. 2a) and Fig. 2b), for two time steps, i.e. t=47.6 s and t=45.6 s. The bubble column clearly changes its position, moving from the left toward the right side of the reactor. The bubble column movement induces the motion of the liquid phase. As already explained before, after 100 s "tracers" have been injected inside the continuous phase in order to simulate the presence of algae. A 1 mm^3 squared volume, centered at the position where the third injection point is located, has been fixed for the simulation of light distribution.
The position of particles has been frozen at the time step t=115.477 s. Fig. 3 shows mutual shading of microalgae. Light enters the domain perpendicular to the x-axis. It can be seen that single cells are shaded by others and consequently receive less light than predicted by an averaged light intensity profile (compare to right side of Fig. 3). At the same time, other cells receive higher light intensities than those predicted by an averaged profile.
Moreover, an exponential model analogous to the Beers-Lambert law fits the averaged simulation data. However, the initial light intensity is overestimated by the model. This indicates that a pure exponential model lacks in accuracy for growth predictions. Similar results are present in literature (Kong et al. 2014).

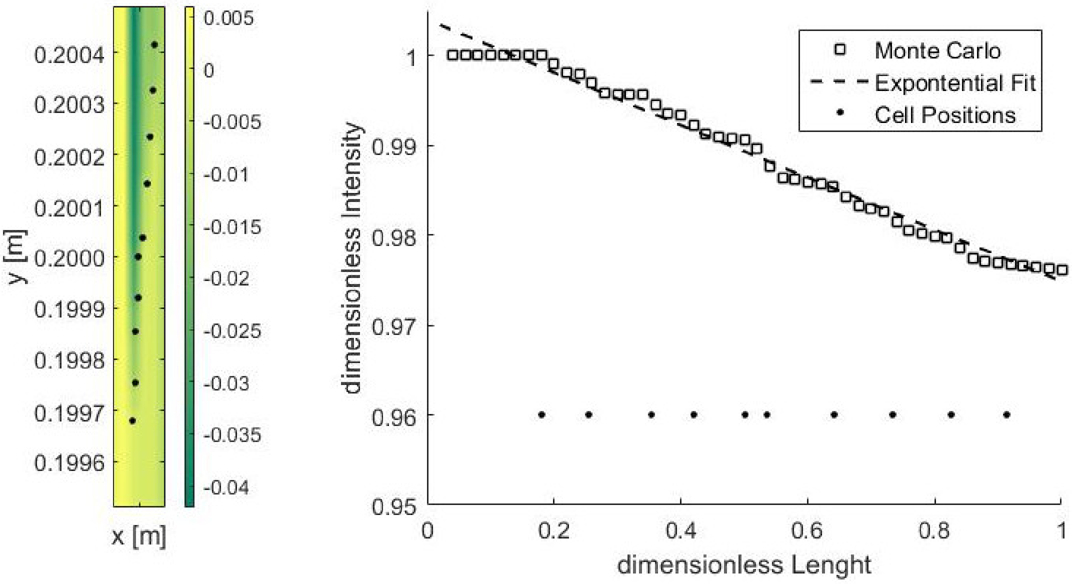

Fig. 3: Contour plot of simulated light intensity distribution. Light enters the domain perpendicular to the x-axis. Spheres symbolize microalgae cells. Color levels, in logarithmic scale, symbolize dimensionless light intensity. Right: Profile of average light intensity along the y-axis. In addition to results from Monte Carlo simulations, an exponential fit according to Beer-Lambert law is shown. Black sphere show cell positions along the light path.

Conclusions

In this work, the bubble column flow inside a bio-reactor has been simulated together with the light distribution inside a 1 mm^3 of the volume, at a specific time step. The numerical simulations successfully reproduce both the oscillating air bubble plume and the shading effects algal cells cause on light, as it passes through a specific region. Nevertheless, more accurate CFD results can be obtained with a finer grid, and a grid independence study needs to be performed.

On the other hand, in order to develop easy-to-use models with high accuracy, further work should address more detailed comparisons of Monte Carlo simulations with macroscopic approximations for light attenuation such as the Beers-Lambert law or the Radiation Transfer Equation (RTE). Moreover, investigating time series of particle positions could give insights to the exposure of single cells to light/dark fluctuations due to velocity gradients in the flow. In the context of microalgae cultivation, these light/dark cycles are known to enhance photosynthetic efficiency and photon yield because of a closer matching of time scales of photon absorption and metabolic conversion (Carvalho 2011).

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