

Comparison of different software for the computation of multiphase flow in photobioreactors

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Abstract

Nowadays a potential choice for a sustainable production of food, feed or fuels is represented by microalgae. The cultivation of these microorganisms often occurs in photobioreactors (PBR) where the maximum allowable culture density is limited to few grams per liters. Enhancing the pneumatic mixing or utilizing different illumination strategies can potentially increase the PBR productivity. In our recent contribution, we compared pneumatic mixing and flashing light illumination with respect to their ability to promote flashing light effects in a 5 cm diameter bubble column PBR. The outcome of our study clearly indicates that at the investigated operating conditions pneumatic mixing alone has no impact at all on the growth rate. In contrast, numerical simulations show that illumination with flashing LED leads to an increase of the growth rate up to a factor of 2.5 at flashing frequencies higher than 50 Hz.

Our numerical work has been conducted with two commercial software, i.e. ANSYS CFX[®] and Matlab[®]. The former one is costly and does not allow much flexibility to modify the source code. In the present contribution, we compare the CFD results for the multiphase flow obtained with ANSYS CFX[®] and OpenFOAM[®], which is a non-commercial software and allows the end user to modify the source codes. The results obtained with the two software match well both qualitatively and quantitatively, demonstrating that OpenFOAM[®] is very robust and can be used to simulate complex processes which are relevant in industry.

Introduction

Turbulent two-phase flows occur frequently in engineering systems. For instance, bubble column reactors are widely employed in chemical process industry and biotechnology. Their strength rely on their unique characteristics, including simple design and competitive investment costs. In addition, they are easy to operate and allow cultivation under conditions of low

shear stress. These features makes PBR attractive for microalgae cultivation. Thereby, microalgae are commonly cultivated in closed PBR where air is supplied to furnish carbon dioxide to the suspension, enable a sufficient mixing and remove oxygen (Olivieri 2014). Therefore, the fluid flow is an important field that has to be determined, since it influences gas liquid mass transfer and mixing, and thus it strongly affects the growth conditions of microorganisms. Consequently, the hydrodynamic characterization of a PBR turn out to be of primary importance and Computational Fluid Dynamics (CFD) is found to be a valid predictive tool compared to costly experimental set-up. Two-dimensional simulations of bubble column flow are computationally much less time consuming compared to three dimensional ones, but they may produce unrealistic results (Mudde and Simonin. 1999), and may strongly depend on the grid size (Bech 2005). Therefore, only three dimensional unsteady computations are able to predict, at least qualitatively, the complex flow patterns of a bubble column PBR (Pfleger and Becker. 2001; Masood and Delgado. 2014). In addition, it is found that the inclusion of all the interphase forces, that is, drag, lift, virtual mass, wall lubrication and turbulent dispersion forces in the numerical model leads to satisfactory results when numerical outcomes are compared to experimental findings (Masood and Delgado. 2014).

Fluid flow in bubble columns have been simulated with both commercial and open source software, like for instance, OpenFOAM®. (Bhusare et al. 2017) analyzed the case of a bubble column with and without internals, comparing their findings with experiments and with numerical results obtained with Fluent®. The numerical results obtained with OpenFOAM® agree well with those obtained with Fluent® and with experiments. (Cheng et al. 2018) performed more sophisticated simulations of a bubble column considering a population balance equation (PBE) to take into account coalescence and break-up phenomena.

In the present contribution, we simulate the two-phase fluid flow inside a bioreactor by means of the open source software OpenFOAM® and we compare the results with our previous findings (McHardy et al. 2018) obtained with the commercial software ANSYS CFX®. Results match very well at different heights inside the column.

Simulation set-up

Geometry and mesh

We consider a cylindrical PBR with an inlet located in one of the bases. The height of the PBR is 50 [cm] and its diameter is 5 [cm]. The diameter of the inlet sparger is 1 [cm]. For both software, we employ the geometry and the mesh we have used in our previous works (McHardy et al. 2018; Luzi et al. 2019). They have been extensively described in (McHardy et al. 2018), therefore they will be briefly mentioned here. Both the geometry and the grid have been generated with the aid of the commercial software ANSYS ICEM®. The domain is covered with a structured grid composed of 54802 volumes.

Mathematical modelling of fluid flow

The mass conservation equation for both phases k may be written as

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

Herein, ρ_k , α_k and \mathbf{u}_k are the density, volume fraction and velocity of each phase, respectively. In Eq. (1) $k = G, L$. L refers to the liquid and G to the gas phase. The momentum equations for both phases read

$$\frac{\partial}{\partial t}(\rho_k \alpha_k \mathbf{u}_k) + \nabla \cdot (\rho_k \alpha_k \mathbf{u}_k \mathbf{u}_k) = \nabla \cdot (\alpha_k \boldsymbol{\tau}_k) - \alpha_k \nabla p + \rho_k \alpha_k \mathbf{g} + \mathbf{M}_{s,k} \quad (2)$$

where, $k = L, G$ again and $s = L, G$ too. The left-hand side of Eq. 2 contains the temporal and the convective acceleration of each phase. The right-hand side incorporates the divergence of the viscous stress tensor of each phase, the pressure gradient, gravity and interphase forces. The stress tensor reads

$$\boldsymbol{\tau}_k = \mu_{k,eff} \left[\nabla \mathbf{u}_k + (\nabla \mathbf{u}_k)^T - \frac{2}{3} \mathbf{I} (\nabla \cdot \mathbf{u}_k) \right] \quad (3)$$

where the effective dynamic viscosity $\mu_{k,eff}$ is the sum of the molecular and the turbulent viscosity, i.e.

$$\mu_{k,eff} = \mu_{k,Lam} + \mu_{k,Turb} \quad (4)$$

The experiments of (Pfleger and Becker. 2001) and (Sokolichin and Eigenberger. 1999) confirm the turbulent character of the liquid flow. They measured the vertical component of the liquid velocity at specific points inside the reactor with the Laser Doppler Anemometry (LDA) technique, in the case of a cylindrical (Pfleger and Becker. 2001) and a rectangular reactor (Sokolichin and Eigenberger. 1999). The velocity of the liquid phase shows random and chaotic variations with time, indicating its turbulent character and therefore the necessity of turbulence modelling. Finally, the term $\mathbf{M}_{s,k}$ in Eq. (2) indicates the averaged interfacial forces. In our simulations, we consider the contribution of the drag, lift, virtual mass, wall lubrication and turbulent dispersion forces. We employ the Grace correlation (Grace et al. 1976) to compute the drag coefficient C_D in ANSYS CFX®, while we apply the Ishii Zuber model (Ishii and Zuber. 1979) to evaluate C_D in OpenFOAM®. The Ishii-Zuber correlation differentiates three bubble regimes, i.e. the spherical bubble, the ellipse distorted and the cap distorted regime. The drag coefficient in the case of the spherical bubble regime reads:

$$C_D(sphere) = \frac{24}{Re_m} (1 + 0.1 Re_m^{0.75}). \quad (5)$$

In the case of the ellipse distorted regime, it is modified as follows:

$$C_D(ellipse) = E(\alpha_\alpha) C_{D\infty} \quad (6)$$

where $C_{D\infty}$ depends on the Eötvös number and on the mixture viscosity.

Finally, the drag coefficient for the cap distorted regime reads:

$$C_D(cap) = \frac{8}{3} (\alpha_L)^2 \quad (7)$$

In the case of the Grace model we have

$$C_D = \alpha_L^f C_{D\infty} \quad (8)$$

where $f = 2$ is a correction factor.

As far as the lift force concerns, we employ the Legendre-Magnaudet model (Legendre and Magnaudet. 1998) to compute the lift force coefficient C_L . It reads

$$C_L = \sqrt{(C_{L,LowRe})^2 + (C_{L,HighRe})^2} \quad (9)$$

Among the interphase forces we also include the virtual mass force which represents the additional mass of liquid added to gas bubbles during their motion inside the PBR. We use a fixed value of the virtual mass coefficient, i.e. $C_{VM} = 0.5$.

With respect to the wall lubrication force, we employ the Frank model to compute the wall lubrication force coefficient C_{WL} (Frank et al. 2004; Frank et al. 2008).

$$C_{WL} = C_W \max \left(0, \frac{1}{C_{WD}} \frac{1 - y_w / (C_{wc} d_B)}{y_w (y_w / (C_{wc} d_B))^{p-1}} \right) \quad (10)$$

where $C_{WD} = 6.8$, $C_{WC} = 10.0$ and $p = 1.7$. C_W is a coefficient that is also function of the Eötvös number.

Finally, we employ the Favre averaged model (Burns et al. 2004) to model the turbulent dispersion forces:

$$\mathbf{F}_{L,G}^{TD} = -\bar{C}_{GL} \frac{\nu_{L,Turb}}{\sigma_{L,Turb}} \left(\frac{1}{\bar{\alpha}_G} + \frac{1}{\bar{\alpha}_L} \right) \nabla \bar{\alpha}_L \quad (11)$$

Turbulence modelling

In order to compute the turbulent eddy viscosity $\mu_{k,Turb}$ of each fluid, we choose the Shear Stress Transport (SST) model (Menter 1994) for the liquid phase and the dispersed phase zero equation for the gas phase in ANSYS CFX®. In case of OpenFOAM®, we selected the mixture $k - \varepsilon$ model for both phases (Bezhadi et al. 2004), since SST is found to be unstable.

Simulation details

The main settings and boundary conditions of the simulations performed with ANSYS CFX® have already been reported in our previous works (McHardy et al. 2018; Luzzi et al. 2019). Therefore, they will not be reported here and space will be allocated to describe the main settings and boundary conditions used in OpenFOAM®. At the inlet location, a value of the gas mass flow rate is specified. At the outlet location, we set the option *pressureInletOutletvelocity* for the velocity field, and *InletOutlet* for the k and ε and the k_m and ε_m fields. In addition, we specify a no-slip boundary condition for the velocity of both fluids, a zero gradient for k_m and ε_m , and the wall functions implemented in OpenFOAM® for both k and ε at the remaining surfaces of the geometry. On the top of the reactor, we leave an air headspace of 10 [cm]. Furthermore, we set a constant fixed mean bubble diameter, $d_B = 7$ [mm] and compare the results between the two software by utilizing the value of gas superficial velocity of $u_G = 5$ [mm/s]. The discretization of gradient, divergence and Laplacian terms of the governing equations is based on Gauss schemes. We solve the Poisson equation of the pressure with the aid of the Geometric-Algebraic Multi-Grid solver implemented in OpenFOAM® with a maximum value of the residual equal to 10^{-8} . In case of the equations of the velocity, k_m and ε_m we choose a slightly looser value of the maximum residual, i.e. 10^{-7} . The coupling between the pressure and the velocity is realized by means of the PIMPLE algorithm, which is a combination of the PISO and SIMPLE algorithms. We set an under-relaxation factor of 0.8 for all the equations. We integrate all the governing equations in time by means of an implicit Euler scheme, which is first order but stable (Bhusare et al. 2017). The selection of the time step is adaptive and it is automatically done based on the maximum value of the Courant number and the maximum value of Δt . Specifically, we set a maximum Courant number of 0.4 and a maximum $\Delta t = 1$ [s]. We run

the simulations up to $t = 300$ [s], a time period which is sufficient for the time averaging (Masood and Delgado. 2014; McHardy et al. 2018)

Results and discussion

In bubble column PBR, air bubbles form a typical meandering “plume”, see for instance Fig. 1 a), and Fig. 1b), at two different time instants. For convenience, the results are displayed on a x-y plane at $z=0$. This bubble “plume” randomly oscillates inside the PBR inducing movements in the liquid phase that are responsible for the mixing mechanism that govern the bubble column hydrodynamics. In addition, the random motion of the liquid phase shuttles algae cells from photic zones of high irradiance level close to the reactor walls to dark ones in the vicinity of the reactor centre. This movements enable the metabolic mechanisms to take place in order to produce the necessary energy for growth and maintenance. Fig. 1 c) shows the streamlines of 1000 tracers ejected from a point close to the inlet after 108.7 [s]. The tracers clearly show strong eddies and recirculation concentrated in the bottom part of the reactor. This happens because close to the inlet the bubble plume is not evenly spread across the cross-section and its vigorous oscillations induces movements on the liquid phase. Fig. 2a) shows the time averaged air volume fraction, computed at $y=0.2$ [m] for the case of $u_g = 5$ [mm/s]. It attains the value of zero at the walls, due to the wall lubrication forces which have the tendency to push the bubbles away from the surface. Therefore, during the oscillations inside the PBR, the bubble column approaches the walls without touching them. Interestingly, the time averaged air volume fraction profile shows two peaks in the vicinity of the lateral surface and a flattened profile in the centre of the PBR. This results is mainly due to the lift and the turbulent dispersion forces: bubbles depart from the centre of the PBR and try to approach the walls but they are pushed back by the wall lubrication forces. It is worth mentioning that the Legendre-Magnaudet model does not consider the sign change of the lift coefficient if the long axis of a deformable bubble exceeds 5.5 [mm]. Instead, this sign change of C_L is taken into account in the

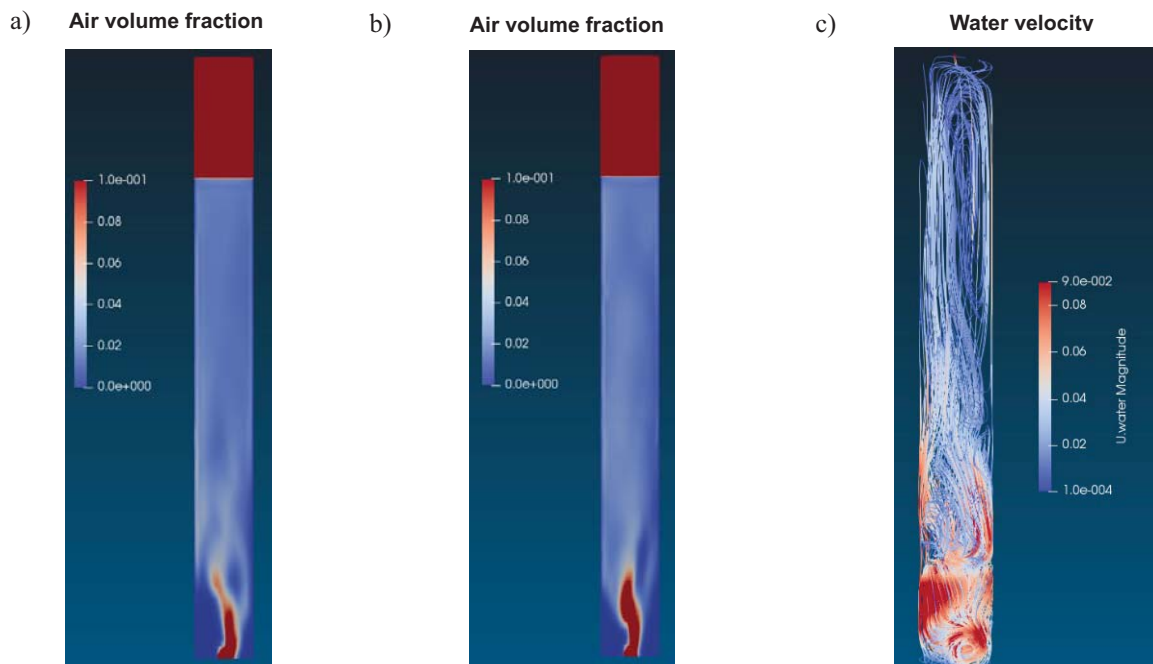


Fig. 1 Air volume fraction on an x-y plane at $z=0$ at $t=65.7$ [s] a) and at $t=117.7$ [s] b). Streamlines of 1000 tracers at $t=108.7$ [s] c). The gas superficial velocity is 5 [mm/s].

Tomiyama model (Tomiyama et al. 2002), which provides an expression for the change of the sign of the lift coefficient based on the long axis of a bubble. A comparison between numerical results obtained with both lift force models is currently under investigation and it is subject of future works. Fig 2b) depicts the profile of the vertical component of the liquid velocity at $y=0.2$ [m]. Numerical simulations correctly reproduce the liquid flow-up at the centre axis and the downward recirculating flow close to the walls. Also in this case, the flattened profile away from the wall is due to the fact that bubbles do not concentrate in the centre of the PBR. On the contrary, they have the tendency to evenly spread inside the column approaching the walls. Finally, we report a comparison between the numerical results obtained with OpenFOAM® and ANSYS CFX®. Specifically, we compare the results of the air volume fraction at two different vertical positions inside the PBR, i.e. at $y=0.05$ [m] and at $y=0.3$ [m]. In the bottom of the reactor, at $y=0.05$ [m], the bubble plume is not yet spread over the entire cross-section of the bubble column, see Fig. 1a) and 1b). Therefore, it is expected that the gas volume fraction reaches a peak in the center of the column and decreases by approaching the reactor walls. It is clear that the numerical results between both software match well both in the bottom and in the top of the reactor, see Fig. 3a) and Fig. 3b). Small differences are mainly due to the different drag and turbulence models used with each software.

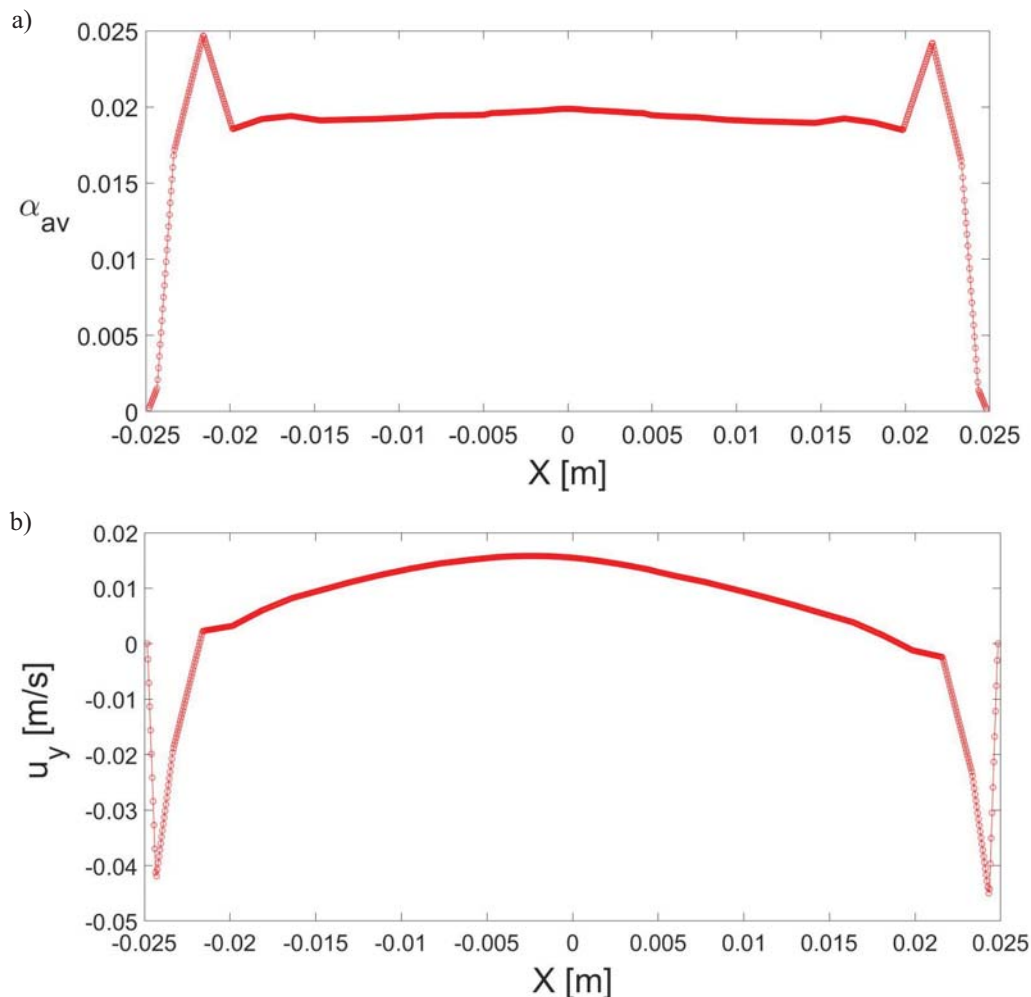


Fig. 2 Time averaged air volume fraction a) and time averaged vertical velocity b) on an x-y plane at $z=0$ at $y=0.2$ [m]. The gas superficial velocity is 5 [mm/s] and the results have been obtained with OpenFOAM®.

In addition, the choice of the discretization schemes and time integration method may also contribute to the deviations. However, they turn out to have a minor impact on the results of the simulations.

Conclusion

In this work, we compared the numerical results obtained with OpenFOAM® and ANSYS CFX® for the case of a cylindrical bubble column PBR operating at low value of gas superficial velocity, i.e. $u_g = 5$ [mm/s]. The simulations show good accordance between both software and the main features of the bubble column flow are successfully reproduced. Those are the meandering bubble plume and the time averaged profiles of air volume fraction and vertical liquid velocity.

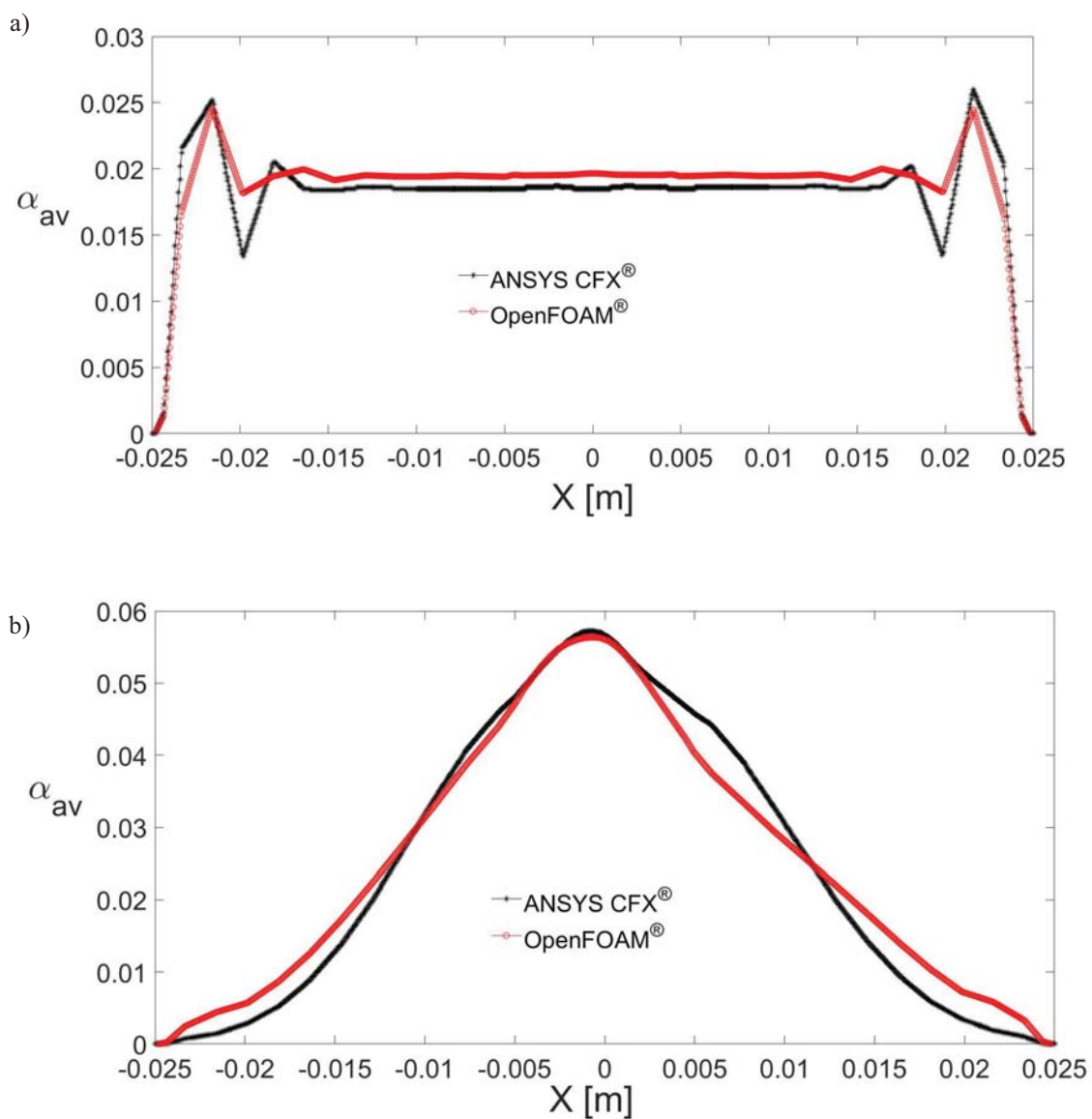


Fig. 3) Time averaged air volume fraction on a x-y plane at $z=0$, $y=0.3$ [m] a) and $y=0.05$ [m] b). The gas superficial velocity is 5 [mm/s]. Red curve: OpenFOAM® results. Black curve: ANSYS CFX® results.

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