

Implementation of a Moments Model in OpenFOAM for Polydispersed Multiphase Flows

João N. E. Carneiro*, Volker Kaufmann, Wolfgang Polifke

*Lehrstuhl für Thermodynamik, TU-München, Boltzmannstr. 15, 85748 Garching,
Germany*

*carneiro@td.mw.tum.de

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Abstract

Accurate simulation of multiphase flows with dispersed particles still represents a great challenge and an open field for research. Examples can be found in several applications such as bubbly flows in aerated stirred vessels, atmospheric aerosols, cloud physics, spray combustion, etc. One of the most important modeling requirements is the ability of capturing the polydispersity in these types of flows. The scope of this work is the further development of a novel approach to simulate multiphase flows with dispersed particles (either droplets or bubbles) based on the moments of the size distribution function (therefore called *Moments Model*). The idea explored here is to use the Eulerian-Eulerian framework (using as a starting point the `twoPhaseEulerFoam` solver), while taking into account the polydispersity by transporting the moments of the particle size distribution function. Each moment is transported with a different velocity (the *moment average velocities*), determined in an approximate manner through a concept using particle relaxation times and force balances. Closure of the moments transport equations is achieved with help of a presumed number density function (pNDF) approach. The *momentum* exchange terms are evaluated using the local instantaneous Sauter Mean Diameter of the size distribution function, providing coupling with the transported moments.

Results presented here – for a test case where buoyancy and (Stokes) drag are considered – show that the model implemented in OpenFOAM is indeed able to capture polydisperse effects efficiently when compared to Multi-Fluid solutions obtained with CFX. For more complex types of interaction (including lift and turbulent dispersion, for example), other closure relations are required, which will be the subject of future work.

1 Introduction

The simulation of polydispersed multiphase flows normally requires a great computational effort with standard techniques. Recently, alternatives to the Lagrangian or the Multi-Fluid approaches have been developed, which makes it possible to account for population dynamics in an efficient manner. Most of these methods rely upon a formulation involving moments (or some other information) of the particle size distribution function, and are divided into three categories: MOM (Method of Moments), QMOM (Quadrature Method of Moments) and DQMOM (Direct Quadrature Method of Moments) [1, 7, 8].

As an open source code, OpenFOAM is a very interesting alternative to commercial CFD solvers for the implementation of models for polydispersed flows (see [10]

for example). The fundamental reason for that is the flexibility to incorporate additional transport equations containing phase independent fluxes within a multiphase flow solver, and the possibility to test different types of formulations for the mass, momentum and energy exchange terms with the continuous phase, as well as different models to compute population dynamics due to break-up, coalescence or phase change, which are highly dependent on the specific application.

The objective of the present work is the implementation of a Moments Model to simulate polydispersed multiphase flows in OpenFOAM, testing it for a simple configuration comprising a channel flow with a dilute mixture of water and air bubbles of different sizes. Results obtained with a simplified closure for the Moments Model are compared with a spectral solution obtained with the Multi-Fluid model in ANSYS-CFX 11.0. Such a test case is particularly interesting once it separates the bubble transport from population dynamics. Hence, it allows to assess the ability of the model to correctly represent the segregation of bubbles with different sizes due to buoyancy effects alone.

2 Model Description

The idea explored here is to use the Eulerian-Eulerian framework of the Two-Fluid Model ([5]), while considering polydispersity by transporting the moments of the particle size distribution function. The moments of the number distribution function $f(D)$ are defined as:

$$M^{(k)} = \int_{D_{min}}^{D_{max}} D^k f(D) dD. \quad (1)$$

A physical interpretation for each of the moments follows:

- $M^{(0)}$: total number of particles (per unit cell-volume)
- $M^{(1)}$: sum of the particle diameter (\parallel)
- $\pi M^{(2)}$: total surface area of particles (\parallel)
- $\frac{\pi}{6} M^{(3)}$: total volume of particles (\parallel); or the local volume fraction of the dispersed phase (α)

The moments transport equations can be written in a generalized form as:

$$\frac{\partial M^{(k)}}{\partial t} + \nabla(u^{(k)} M^{(k)}) = S_{M^{(k)}}, \quad (2)$$

with $S_{M^{(k)}}$ the source terms resulting from the population balance dynamics. The moment average velocities $u^{(k)}$'s (averaged over the k^{th} moment) appearing in Eq. (2) are in turn given by:

$$u^{(k)} = \frac{1}{M^{(k)}} \int_{D_{min}}^{D_{max}} u D^k f(D) dD, \quad (3)$$

which are the mean velocities at which the moments are convected¹. There is no reason, e.g., for $u^{(2)}$ and $u^{(3)}$ to be the same, as they are surface area and mass

¹Implicit here is the assumption that particles with the same size have at a given location the same velocity, i.e., $f = f(D, x, t)$, and not $f = f(D, u, x, t)$

averaged velocities, respectively. Moreover, except for $u^{(3)}$, which actually is determined by the dispersed phase momentum equation, none of the $u^{(k)}$'s is known *a priori*. Therefore, some modeling effort is needed at this point².

The ‘‘Equilibrium Eulerian method’’ was introduced in [3, 4]. In the limit of very small particle relaxation times, particle terminal velocity deviates very little from the continuous phase velocity, scaling with the first order of the relaxation time. On the light of this idea, Bollweg et al. [2] propose a linear interpolation between the continuous phase and reference particle velocities (with size larger than minor groups) to determine minor particle size velocities. Here, we make use of this approximation in order to derive relations for the determination of moment average velocities from known velocities, thus allowing the development of a closure for Eq. (2).

In the present study, the driving force which leads to the segregation of bubbles with different sizes results from a balance between drag and buoyancy. The Lagrangian equation of motion for each particle can be written in this case as:

$$\frac{du_{r,i}}{dt} = \frac{1}{\tau_i}(u_{T,i} - u_{r,i}), \quad (4)$$

with the relaxation time τ_i (assuming Stokes Flow) defined as

$$\tau_i = \frac{\rho_d D_i^2}{18\mu_c}, \quad (5)$$

$u_{r,i}$ and $u_{T,i}$ are the relative and terminal velocity of bubble class i , respectively. They are in turn defined as:

$$u_{r,i} = u_i - u_c \quad (6)$$

and

$$u_{T,i} = \frac{\Delta\rho g D_i^2}{18\mu_c}, \quad (7)$$

with $\Delta\rho = \rho_d - \rho_c$. By using the approximation proposed in [2], and integrating over the particle spectrum, it is possible to write:

$$u^{(k)} = u_c + u_T^{(k)} - \frac{\tau^{(k)}}{\tau_0}(u_c - u_0 + u_{T,0}), \quad (8)$$

for the interpolation of moment average velocities with $k \leq 2$. In the above equation, the averaged particle relaxation time $\tau^{(k)}$ is defined as:

$$\tau^{(k)} = \frac{1}{M^{(k)}} \int_{D_{min}}^{D_{max}} \tau D^k f(D) dD, \quad (9)$$

and the index 0 refers to reference properties used in the interpolation procedure. Since $M^{(3)}$ and $u^{(3)}$ are given by the solution of the continuity and momentum equations, they are primary candidates for reference properties. This approximation will show to be sufficient for the present purposes, but can not be expected to be valid in a broader context, e.g. if Stokes approximation is no longer valid or non-drag forces are considered. This will be subject of future investigation.

By introducing Eq. (5) into (9), it is possible to write:

$$\tau^{(k)} \propto \frac{M^{(k+2)}}{M^{(k)}}. \quad (10)$$

²In fact, averaged equations can be formulated for each $u^{(k)}$, by integrating the dispersed phase momentum equations over the size spectrum, but this is out of the scope here

From the moments transport equation (2) – setting for simplicity the source term to null– and with help of relation (8), it follows that:

$$\frac{\partial M^{(k)}}{\partial t} + \nabla(u_c M^{(k)}) = \nabla \left[\underbrace{(u_c - u^{(k)})}_{\frac{\tau^{(k)}}{\tau_0}(u_c - u_0)} M^{(k)} \right] \quad (11)$$

If Eq. (10) is substituted into (11), it follows that to determine a certain lower order moment $M^{(k)}$, $M^{(k+2)}$ must be known. This gives rise to a closure problem.

A simple way to overcome this issue is to assume the functional form of $f(D)$ (a presumed Number Density Function – pNDF), calculating unknown moments by reconstruction of the distribution using lower order moments. Here, we choose the Gamma distribution function, as it is able to represent a wide variety of size distribution spectra. Furthermore, its reconstruction from lower order moments is straightforward, making it very suitable for the present purposes (although other functional forms can be easily incorporated in the model). Hence, if $f(D)$ is given by a Gamma function:

$$f(D) = C_0 \frac{D^{\beta-1} e^{-\frac{D}{\alpha}}}{\alpha^\beta \Gamma(\beta)} \quad (12)$$

with

$$\begin{aligned} C_0 &= M^{(0)} \\ \alpha &= \frac{M^{(2)}M^{(0)} - (M^{(1)})^2}{M^{(0)}M^{(1)}} \\ \beta &= \frac{(M^{(1)})^2}{M^{(2)}M^{(0)} - (M^{(1)})^2}, \end{aligned} \quad (13)$$

any higher order moments can be explicitly calculated as:

$$M^{(k)} = C_0 \frac{\Gamma(\beta + k) \alpha^k}{\Gamma(\beta)}, \quad k \geq 3. \quad (14)$$

The complete model requires the solution of Eq. (2) for $M^{(0)}$ - $M^{(3)}$, with $M^{(4)}$ given by Eq. (14). The solution of the coupled moments transport equations enables the calculation of the Sauter Mean Diameter of the distribution, determined by $D_{32} = \frac{M^{(3)}}{M^{(2)}}$. This mean diameter is in turn used to calculate the effective drag used in the phase momentum equations, hence providing coupling to the moments equations.

3 Implementation in OpenFOAM

OpenFOAM is a C++ class library which can be easily used to develop CFD codes for a wide variety of problems, including multiphase flows, either by starting from existing solvers or by developing completely new ones, using capabilities of the finite volume method already available [6, 12].

The objective here is to illustrate the incorporation of additional transport equations for the moments within a two-phase flow solver using a simple closure for $u^{(k)}$ through a concept using relaxation times and force balances, as illustrated above.

The solution of additional transport equations for the moments within the `twoPhaseEulerFoam`³ is done following the pressure-velocity system, as it would be the case of the $k - \epsilon$ equations, for example. Regarding the implementation in the code itself, the moments transport equations can be defined within the tensor derivative class `fvScalarMatrix`, with all terms being treated implicitly through the class `fvm`, as depicted by the following code snippet:

```
surfaceScalarField C = tauk*(phib-phia)/taua;

fvScalarMatrix mkEqn
(
    fvm::ddt(mk)
    + fvm::div(phib, mk)
    + fvm::div(C, mk) //convective correction
);

mkEqn.relax();
mkEqn.solve();
```

According to Weller's notation [11], the discretised form of the moments transport equations is given by:

$$\left[\frac{\partial [M^{(k)}]}{\partial t} \right] + \left[\nabla \cdot (\phi_b [M^{(k)}]_{f(\phi_b, UD)}) \right] + \left[\nabla \cdot (C [M^{(k)}]_{f(C, UD)}) \right] = 0, \quad (15)$$

where the Euler implicit scheme for the time derivative and upwind differencing face values of $M^{(k)}$'s for the convective terms were used. The relaxation times `taua` and `tauk` for the correction coefficient `C` are defined as `surfaceScalarField` types, given by Eqs. (5) – calculated using the Sauter Mean Diameter – and (10). Thus, segregation of the moments throughout the flow field is achieved by considering different convective corrections for each transport equation. Moreover, coupling with the phase equations is achieved through the drag force, where the dispersed phase diameter is simply the updated value of the Sauter Mean Diameter through use of the pNDF approach described earlier.

4 Test Case

The channel flow represents a simple configuration which allows to assess the ability of the model to predict effects of polydispersity due to buoyancy through convection of the moments in the flow field. The set up consists of a channel with 2 cm height and 10 cm length. A dilute mixture of water and air bubbles at standard conditions was considered. The dispersed phase volume fraction at the inlet corresponded to 10^{-5} and the mixture Reynolds number was chosen to be approximately 2000. A constant pressure was kept at the outlet, with zero gradient boundary conditions for all other variables. For simplicity, slip conditions at the walls were applied, in order to avoid accumulation of bubbles at the top wall. Boundary conditions for the moments were taken from the size distribution function applied to the Multi-Fluid case, which is shown in Fig. (1). The range of sizes considered was 10-150 μm , with a total of 15 bubble size classes and maximum particle Reynolds number with order of magnitude of 1.

³A full description of the Two-Fluid Model implemented in OpenFOAM can be found in [9].

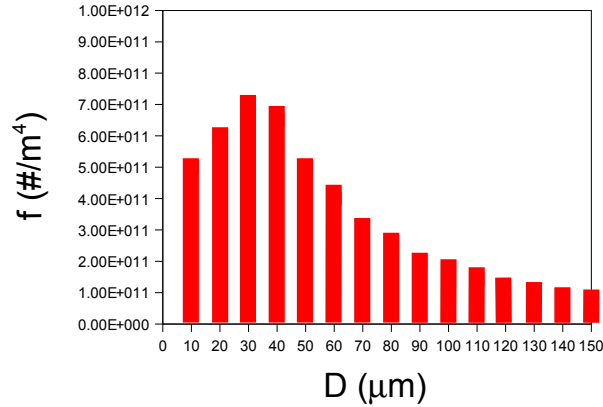


Figure 1: Initial Distribution used in the spectral case.

The simulations were carried out with a 2D hexahedral mesh of 50x150 points and a fixed time step of 10^{-5} s. For the solution of the discretised equations, the pre-conditioned (bi-) conjugate gradient linear solvers were used, with a convergence criteria of 10^{-10} for both pressure and volume fraction.

Figure (2) shows the distribution of the Sauter Mean Diameter inside the channel obtained with the Moments Model in OpenFOAM. An increase towards the upper wall can be clearly observed. This reflects the fact that the vertical velocity induced by buoyancy tends to increase with the bubble diameter. Since the contribution of bigger bubbles becomes more important for higher order moments, $M^{(3)}$ rises faster than $M^{(2)}$, leading consequently to an increase in D_{32} .

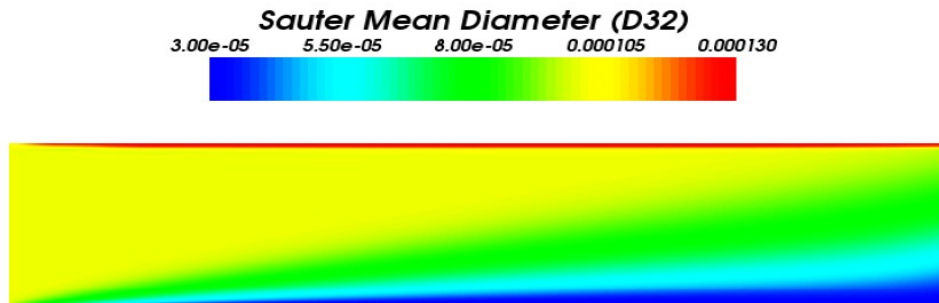


Figure 2: Contours of the Sauter Mean Diameter obtained with the Moments Model in OpenFOAM.

Simulations were also performed with the Multi-Fluid Model available in ANSYS CFX 11.0 and used as a reference solution to validate the Moments Model implemented in OpenFOAM. Thus, sets of conservation equations for mass and momentum were solved for the Eulerian phases (a total of 15 dispersed phases and 1 continuous phase), and the post-processed local particle size distribution function, as well as all its moments, were compared to the solution obtained with the Moments Model.

The axial evolution of the moments (normalized by the inlet values) at both walls is shown in Fig. (3) for both cases. The overall behavior is well represented

by the Moments Model, also comparing quantitatively well against the Multi-Fluid approach: as bigger bubbles tend to migrate faster to the upper side of the channel, higher moments tend to decrease faster at the bottom wall and increase faster at the top wall.

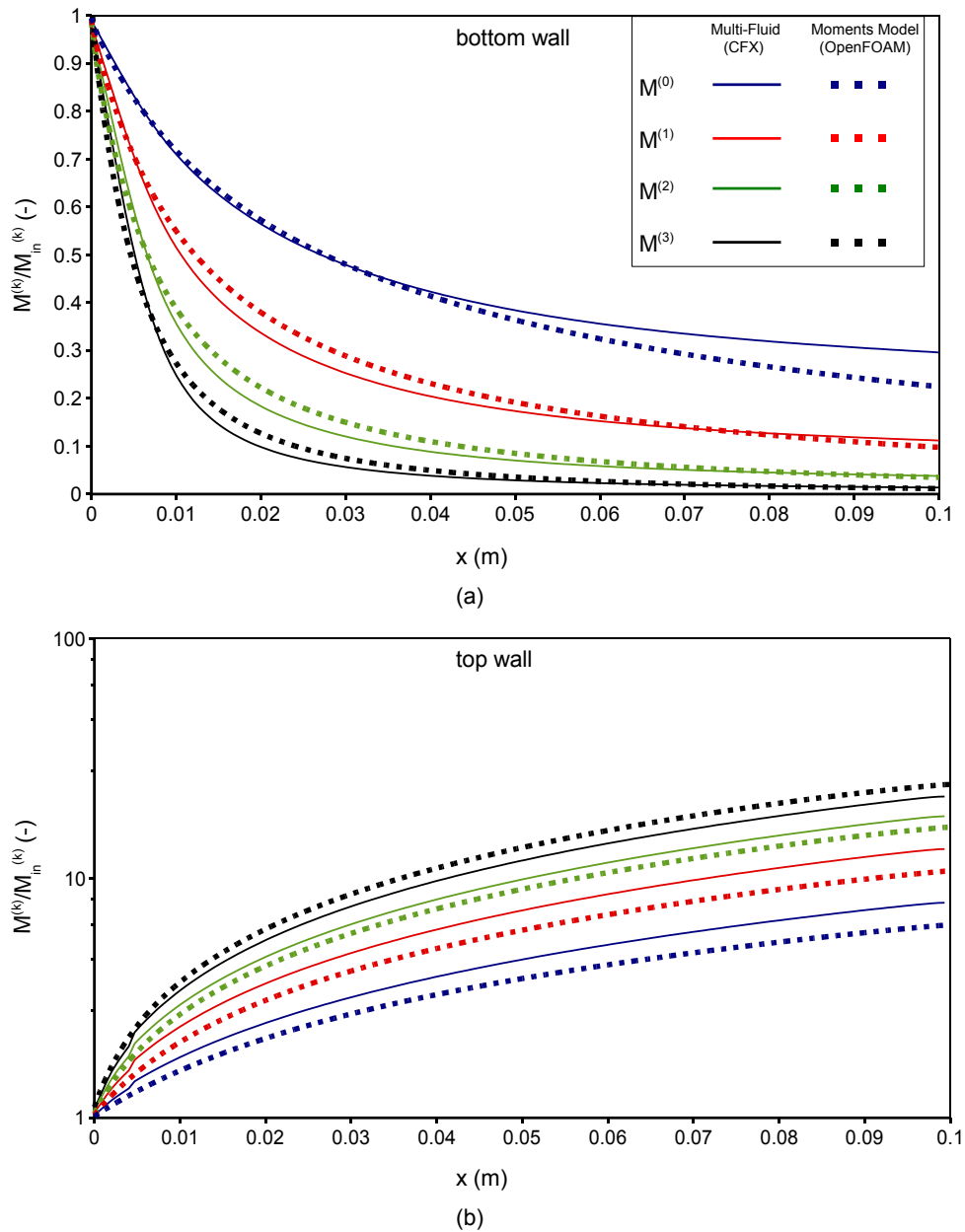


Figure 3: Comparison of the evolution of the normalized moments along the channel at the bottom (a) and top (b) walls.

Figure (4) shows the evolution of the bubble size distribution function at several positions inside the channel (corresponding to axial positions $x = 1,5; 5,7$ cm and vertical positions $y = 0,1; 10; 19,9$ mm). As bubbles tend to move towards the upper side of the channel, the number density is higher for the vertical coordinate corresponding to $y = 19,9$ mm, and smaller at $y = 0,1$ mm. Furthermore, a very reasonable agreement can be noted between both methods, with the Moments Model being able to reproduce not only the shape of the distribution function, but also its

variation along the channel. However, the distribution obtained with the Moments Model near the upper wall at the most downstream axial position in the channel deviates considerably from that of the Multi-Fluid solution. This occurs because the shape of the spectral distribution at that location is dominated by the high accumulation of big bubbles near the top wall, which is not appropriately reproduced by a Gamma distribution.

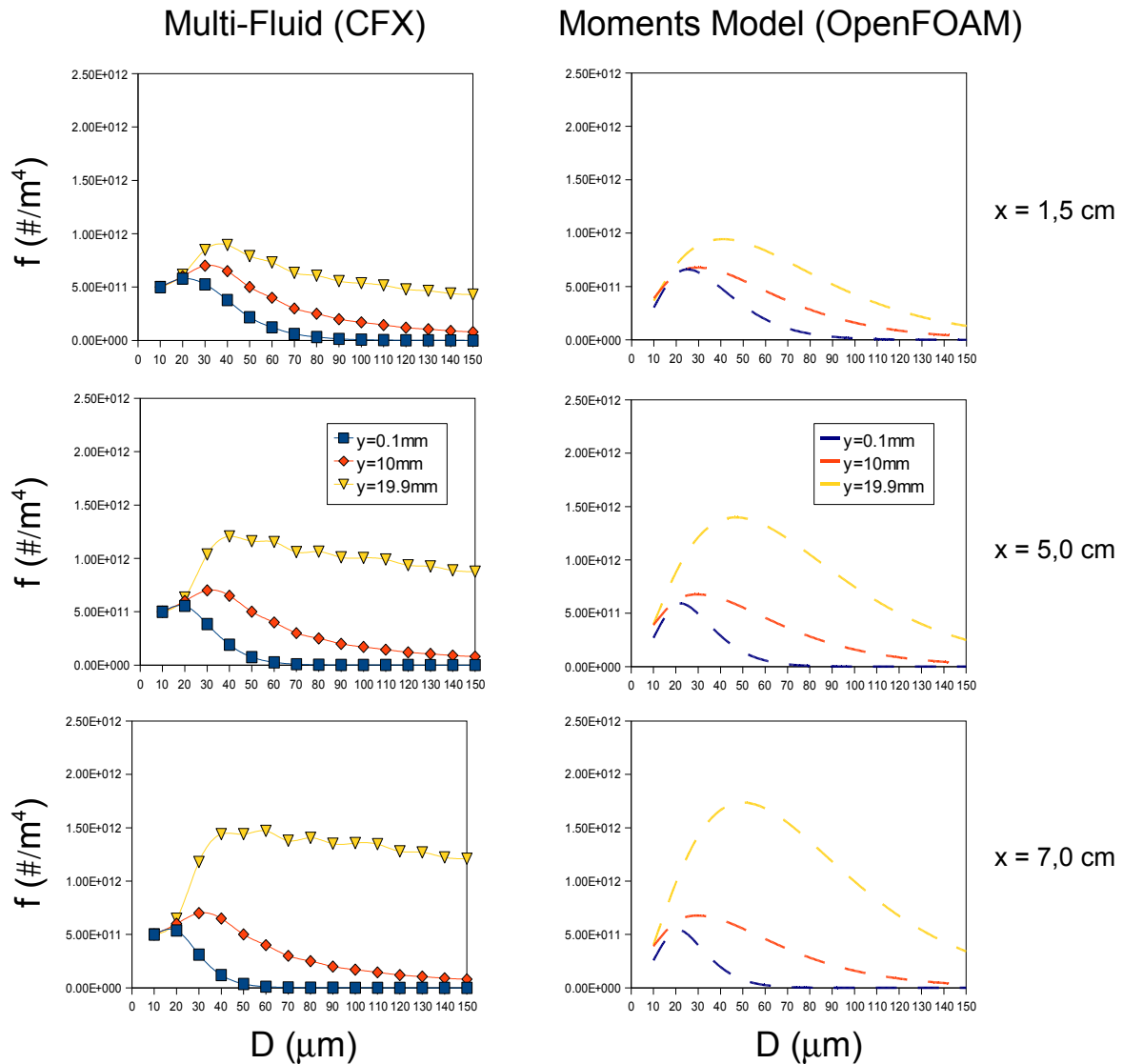


Figure 4: Comparison of the evolution of the bubble size distribution function along the channel.

5 Conclusions and Future Work

A new Moments Model for polydispersed multiphase flows with a simplified closure for the moment average velocities was presented and its implementation within the `twoPhaseEulerFoam` solver of OpenFOAM was illustrated. The model was tested

for a simple configuration comprising of a channel flow with a two-phase mixture of water and air bubbles. Very reasonable agreement for the evolution of the bubble size distribution function and its moments inside the channel was obtained against simulations carried out with the Multi-Fluid Model available in ANSYS CFX 11.0, showing that the model was able to capture effects of polydispersity due to buoyancy. It is clear, however, that a correct description of the polydispersity hinges on the determination of $u^{(k)}$, which was done here in an approximate manner through a concept using particle relaxation times and force balances. The further development of the model involves the implementation of extra averaged momentum equations to determine the moment average velocities, with special closure needed to treat other types of interactions (e.g., lift and turbulent dispersion forces). OpenFOAM has proven to be a very appropriate tool for this task.

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