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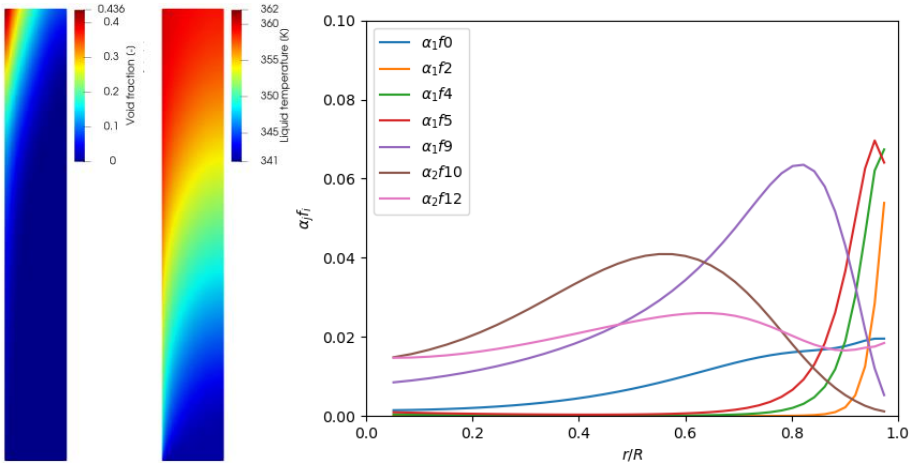

On modelling of turbulent dispersion in polydisperse flows

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Summary

This report serves as a summary for the findings related to polydisperse flow modelling in the SAFER2028_CERESA_2023 project. We report that the present capabilities of OpenFOAM population balancing model are not fully sufficient for Reynolds Averaged Navier-Stokes (RANS) modelling of turbulent polydisperse multiphase flows. In particular, we demonstrate that the effect of modelled turbulence is not properly taken into account in the transport of the population balance size group fractions leading to misprediction of bubble size distribution. Similar transport formulations are also used in inhomogeneous class method population balance models of other widely used CFD codes. We note that in practical industrial applications, the majority (if not all) of the turbulence is typically modelled and as such turbulent dispersion effects cannot be resolved in the simulation and instead need to be modelled. The underlying core issues are explored, and modifications are proposed to the numerical implementation of the transport equations which would allow to more correctly represent turbulent dispersion of the different size groups.

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1. Introduction

Computational Fluid Dynamics (CFD) has previously been successfully applied in nuclear safety assessment, which involves comprehensive evaluation of various factors, including thermal-hydraulic performance, containment integrity, and the behaviour of radioactive substances under different operating conditions. Traditional experimental methods are often limited in their ability to capture the intricate details of fluid dynamics in complex geometries within nuclear reactors and other related systems. This is where CFD simulations have proven to be useful. CFD simulations can provide a detailed understanding of the thermal-hydraulic behaviour within reactor cores, coolant systems and containment structures. This information is crucial for assessing the safety margins and identifying potential vulnerabilities in the event of various operational and accident scenarios.

Studies related to containment structures, in particular, involve modelling of phenomena, in which the transport of particles of different sizes is essential. Examples of such include the modelling of sprays, aerosol transport and boiling. In the context of severe accidents, CFD simulations play a vital role in predicting the behaviour of released radioactive materials, facilitating emergency response planning, and mitigating potential consequences. Understanding the dispersion patterns and transport mechanisms of airborne contaminants under various accident scenarios is essential for developing effective emergency response strategies and ensuring the safety of both plant personnel and the public at large.

To properly describe complex interlinked phenomena, such as the inter-phase forces in a multiphase system, their effect on the flow, and the resulting heat and mass transfer, multiple closure models need to be included in the CFD model to handle the individual phenomena and their interconnections. The selection of suitable closure models is often difficult since the behaviour of the model combination is hard to predict due to the interconnections between the different physical models. Furthermore, many closure models contain model parameters, which ideally should be fitted against suitable experimental data. However, it is often difficult to discern which model is responsible for a certain effect, or even to predict how or which way the results change when a certain parameter is tuned, or a different closure model is selected. This becomes painfully obvious when attempting to validate a complex CFD model against experiments conducted in an integral test facility where multiple phenomena occur at the same time.

The aspects discussed above highlight the importance of continuous model development and validation efforts on reducing the uncertainties inherent in computational modelling, which ultimately lead to improved reliability of nuclear safety assessment.

2. Debora benchmark

The DEBORA facility at CEA-Grenoble focused on high-pressure flow boiling in a simple vertical tube geometry. To mimic the high-pressure conditions relevant for nuclear safety related applications in Pressurized Water Reactors, freon (R12 or R134a) was used as the working fluid. The DEBORA benchmark consists of several tests conducted with the DEBORA facility. The benchmark cases have two defining characteristics in common: (1) most of the void is created as relatively small bubbles ion the surface of a heated wall and (2) there is a rapid change in bubble diameter near the wall. Looking at the interfacial forces typically implemented in a state-of-the-art, inhomogeneous polydisperse bubbly flow model, there are only two pathways that can lead to the development of a centre channel void peak. Either the small bubbles near the wall need to coalesce and move to the large bubble group (where the lift force points towards the centre of the channel) or disperse towards the centre of the channel (against the lift force). With the small nucleate bubbles, commonly applied wall lubrication models are insignificant in the near wall region.

The near wall void peak is relatively straight-forward to reproduce with a set of well-established closure models. However, it should be possible to predict both the near wall and centre channel void peak, and

the transition between them, with the same model, which is so far, at least for the authors' knowledge, beyond the reach of any set of selected closure models or modelling approaches applicable to practical nuclear safety assessment studies.

A typical, state-of-the-art, inhomogeneous polydisperse bubbly flow model is exemplified by the implementation found in OpenFOAM 11 (OpenFOAM Foundation, 2023) multiphaseEuler solver module. In an inhomogeneous model, the dispersed phase is split into velocity groups that share a common transport velocity. Typical choice is one velocity group for large and one for small bubbles.

In the implementation, turbulent dispersion only affects the bulk motion of the velocity group (since the turbulent dispersion force is relative to the gradient of velocity group's volume fraction). Transport of size groups is unaffected beyond the bulk motion of the whole velocity group. The same limitation applies to all the interfacial forces, but the turbulent dispersion is uniquely affected because of its sensitivity to volume fraction gradient. With one velocity group this affects the modelling of bubble size, but with multiple velocity groups the simulation results can be sensitive to the selected number of velocity groups and the chosen diameters at which the divisions between the groups occur. Furthermore, it is difficult to suggest a sufficient value for the number of velocity groups as with a given set of interfacial models, the total amount of dispersion increases as the number of velocity groups increases, or even to justify the need for more than (one or) two velocity groups.

These observations led to detailed investigation of the underlying issues in turbulent dispersion modelling with polydisperse flows, which is described in the following chapters.

An overview of the results for a previously published DEBORA case, which is also included in the OpenFOAM Foundation's release as a tutorial case, is presented in Figure 1. The heated wall is on the left side of the domain and the centre of the channel is on the right side. Significant void fraction, and a steep gradient in void fraction, is visible near the heated wall close to the channel outlet (top). Net phase change, shown on the right side of Figure 1, is a combination of wall nucleation and interface phase change between the vapor and liquid phases. Right next to the wall is a thin red line where nucleation occurs. The condensation caused by the subcooled liquid is visible as the blue patch (negative values) close to the heated wall, roughly half-way up the channel. Large positive values are visible near the wall at the end of the channel.

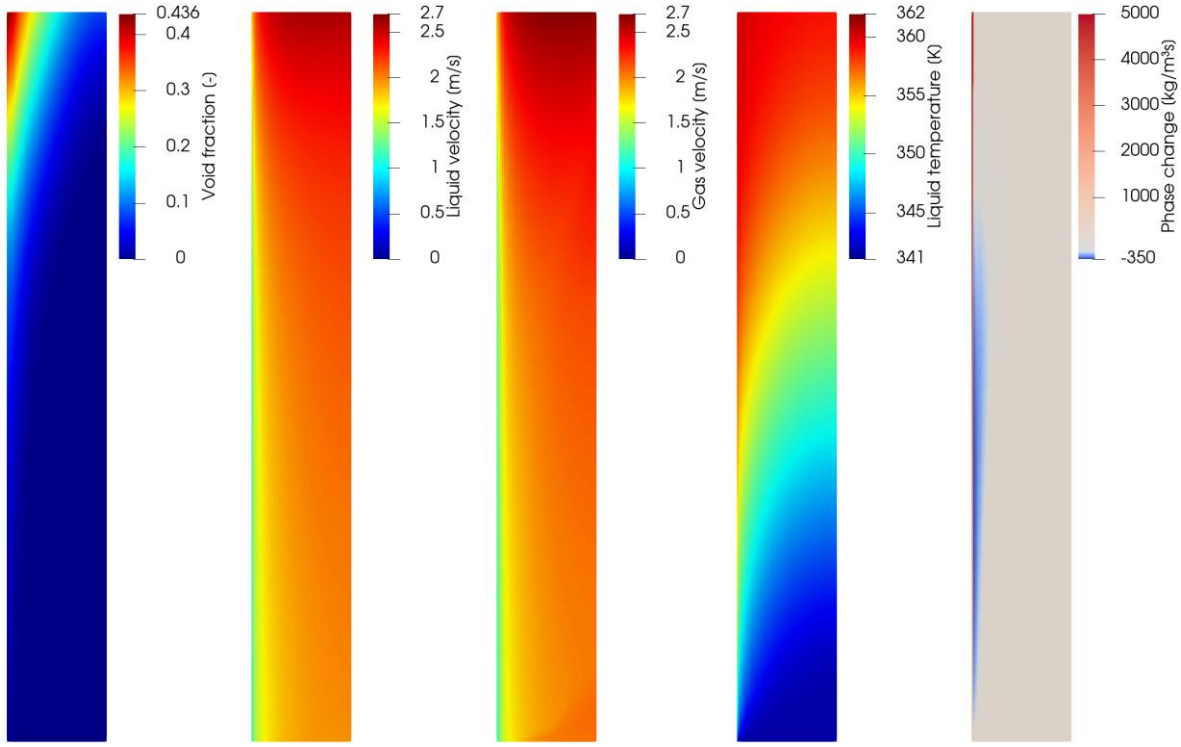

Figure 1. Overview of results for void fraction, velocities, liquid temperature and net phase change mass flux. Geometry has been vertically scaled 1:50 for visualization purposes. The heated wall is on the left side of the domain. Results shown are from OpenFOAM `wallBoilingPolydisperseTwoGroups` *tutorial.*

A comparison of simulation results to experimental measurements at the end of the heated section is given in Figure 2 for three available variables: void fraction [-] (top left), liquid temperature [K] (top right) and Sauter mean diameter [mm] (bottom left). Mass balance monitors have been added for reference on the bottom right corner of Figure 2. Notice the steep gradient in both near wall void fraction and Sauter mean diameter.

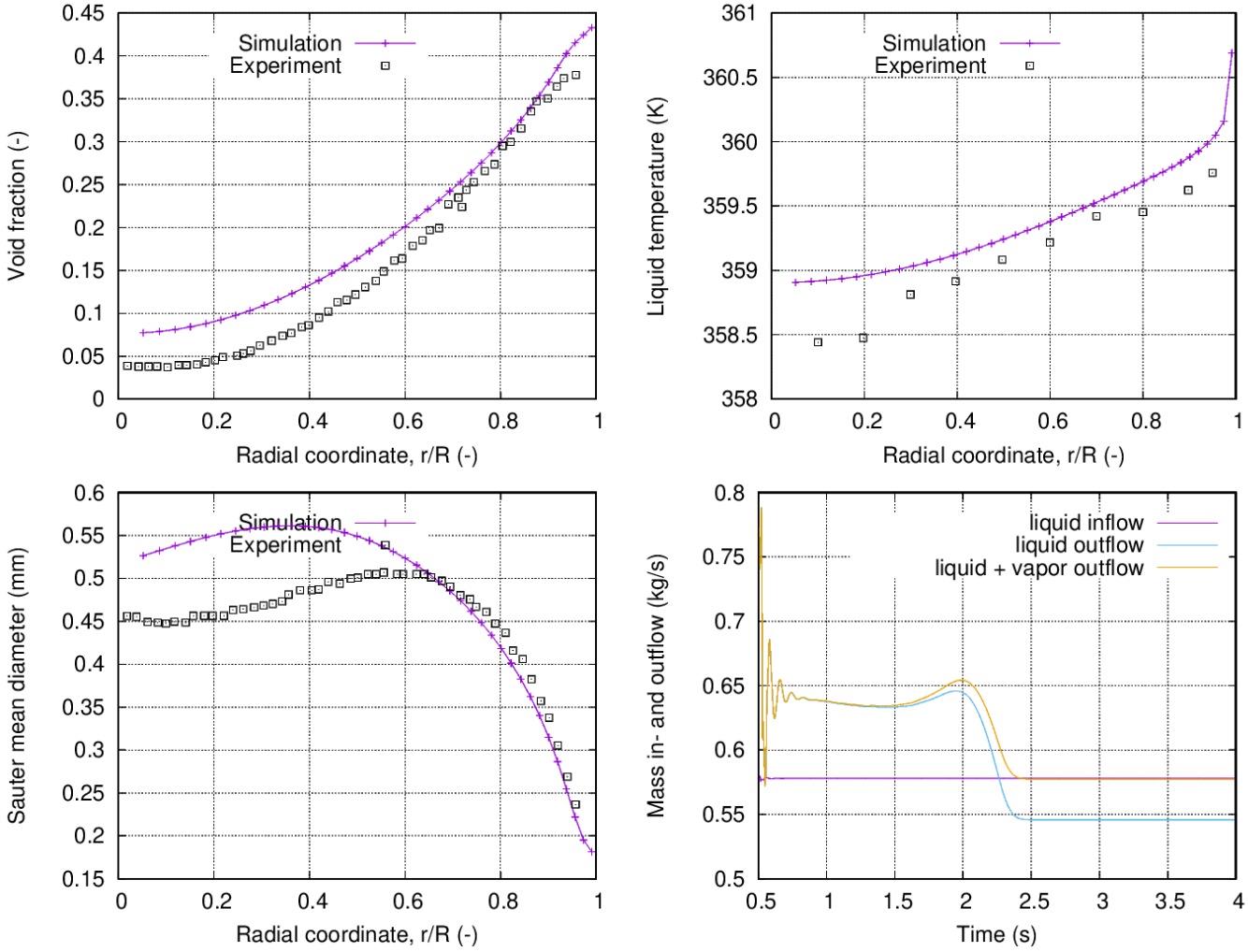

Figure 2. Comparison of simulation to experimental results and mass balance monitors during the simulation from tutorial `wallBoilingPolydisperseTwoGroups`*.*

Radial profiles of void fractions of selected size groups are presented in Figure 3. Size groups f0 to f9 belong to the “small bubble” velocity group and the rest belong to the “large bubble” velocity group. The division between the velocity groups is made based on the sign of the lift force; the small bubbles are drawn towards the wall (right) and the large bubbles are pushed towards the centre of the channel (left). From the figure it can be noticed how the gradient of the profiles is opposite near the wall for size groups f0 and f9, which both belong to the same velocity group. This indicates that turbulent dispersion should spread these groups in opposite directions near the heated wall. In the current form, the turbulent dispersion models do not account for this.

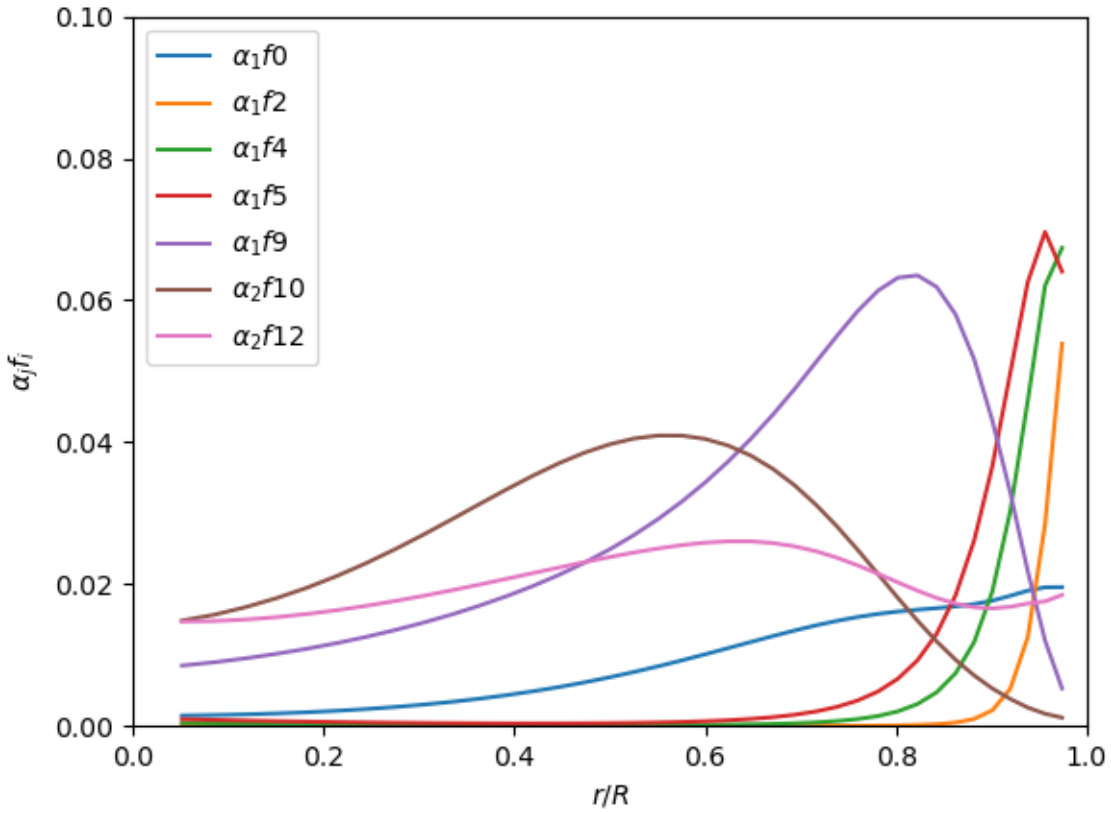

Figure 3. Volume concentrations of selected size groups at the end of the heated section. Size groups f0 to f9 belong to the "small bubble" phase.

3. Modelling of polydisperse multiphase flow

Various applications in industrial fluid flow deal with secondary phases that include particles of different sizes. The size distribution of particles, such as bubbles, droplets, or solid particles, can evolve due to chemical reactions or other processes as they are transported in a multiphase system. These processes involve various phenomena such as nucleation, growth, dispersion, dissolution, aggregation, and breakage. Therefore, in multiphase flows with a size distribution, it is necessary to formulate a balance equation that considers the alterations in the particle population. This equation is commonly known as the population balance equation (PBE). Instances where a population balance may be applicable include bubble columns, gas sparging, sprays, crystallization, precipitation and granulation, among others.

The population balance equation is typically formulated as a transport equation with integral source terms making it a rather complicated integro-differential equation. For practical numerical solution especially in CFD context, it needs to be efficiently discretized. There are multiple ways how this can be done, but two commonly adapted approaches are the Quadrature-based method of moments (QMOM) and the method of classes.

In the OpenFOAM Foundation release a class method is implemented. The approach is very briefly described here, but a more detailed description of the implementation is given in PhD Thesis of the main author of the model Lehnigk (2020) and Lehnigk et al. (2021). The implemented model uses fixed pivot technique described by Kumar & Ramkrishna (1996).

In a class method the particle size distribution is discretized into a number of separate size groups and for each size group a separate discretized PBE equation is solved. The PBEs are formulated in terms of number densities N_i of each size group which yields following transport equations

$$\frac{\partial N_i}{\partial t} + \nabla \cdot (\boldsymbol{U}_d N_i) = H_i \tag{1}$$

Under Eulerian multiphase framework, it is more convenient to express the amounts in terms of volume concentrations

$$\alpha_i = v_i N_i \tag{2}$$

where v_i is a representative particle volume. When summed over all the size groups, the volume concentrations should yield a total volume fraction α_d of a dispersed phase d,

$$\alpha_d = \sum \alpha_i \tag{3}$$

In principle the volume fraction of a dispersed phase could be derived from the transport equations of the individual size groups. However, in practice the population balance model is considered to be an “addon” to the general purpose *multiphaseEuler* solver and the total dispersed phase volume fraction is considered to be a fundamental variable which is solved before the PBEs. The role of the population balance model is then to solve how the dispersed phase elements are distributed with respect to size given an overall volume fraction α_d. To enable this, the PBE equations are further transformed into equations for size group fractions f_i

$$f_i = \frac{\alpha_i}{\alpha_d} \tag{4}$$

These fractions should be bounded between zero and one and sum up to unity

$$0 \leq f_i \leq 1, \qquad \sum_i f_i = 1 \tag{5}$$

When Equation (1) is expressed in terms of size group fractions, it becomes

$$\frac{\partial \alpha_d f_i}{\partial t} + \nabla \cdot (\alpha_d \boldsymbol{U}_d f_i) = S_{ij} \tag{6}$$

S_{ij} are the sources (coalescence, breakup, mass transfer, density change) describing transfer of particles from size group to another. This is the form (together with some numerical stability terms) which is implemented in the OpenFOAM solver.

In the basic, or homogeneous class method, only one dispersed phase is used to represent the entire distribution, and this means that all the size groups would share a common velocity. This approximation can be quite limiting, as in many flows the size strongly affects the forces affecting a particle and thus differently sized elements would travel at different velocities. To improve over the homogeneous class method, in the inhomogeneous class method, a single physical phase can be divided into any number of so-called velocity groups which are then divided into size groups. At solver level velocity groups are like any other phases and for each of them a momentum equation and separate velocity field is obtained. Internally the population balance model keeps track which velocity groups belong to a single population balance and keeps track of all the size groups in all velocity groups.

With multiple velocity groups, the interpretation is that the multiple velocity groups, i.e. phases α_φ represent a single, physical dispersed phase α_d such that

$$\alpha_d = \sum_{\varphi \in d} \alpha_\varphi \tag{7}$$

and the size fractions are redefined as

$$f_{i,\varphi} = \frac{f_i \alpha_d}{\alpha_\varphi} \tag{8}$$

For each size group in each velocity group a transport equation, equivalent to Equation (6), is solved

$$\frac{\partial \alpha_\varphi f_{i,\varphi}}{\partial t} + \nabla \cdot \left(\alpha_\varphi \boldsymbol{U}_\varphi f_{i\,\varphi}\right) = S_{ij,\varphi} \tag{9}$$

In this case the basic form is the same as in Equation (6), but the source terms also contain transfer of particles between velocity groups with special handling for those size groups that lie next the interface between the velocity groups.

From a physical point of view, the best representation would be achieved by using a single velocity group for each size group. However, in practice adding many velocity groups quickly increases the computational costs of the simulation and adds complexity to the case setup. Thus, only a few velocity groups (e.g. between 1-4) are commonly used. Individual size groups are much less computationally expensive than velocity groups and typically at least tens of size groups can be used.

4. Turbulent dispersion and OpenFOAM class method population balance model

4.1 Turbulent dispersion in multiphase flows

In Eulerian multiphase simulations the basic flow equations solved for each phase are the continuity equation and momentum transport equations. The continuity equation for phase φ can be written as

$$\frac{\partial \alpha_\varphi \rho_\varphi}{\partial t} + \nabla \cdot \left(\alpha_\varphi \rho_\varphi \boldsymbol{U}_\varphi\right) = \mathrm{S}_\varphi \tag{10}$$

where α_φ is the volume fraction and ρ_φ the density of the phase and S_φ are source terms such as mass transfer in an out of the phase or possible user-defined mass source terms. The momentum transport equation is

$$\frac{\partial \alpha_\varphi \rho_\varphi \boldsymbol{U}_\varphi}{\partial t} + \nabla \cdot \left(\alpha_\varphi \rho_\varphi \boldsymbol{U}_\varphi \boldsymbol{U}_\varphi\right) + \boldsymbol{R_\varphi} = \boldsymbol{M}_\varphi + \boldsymbol{S}_U \tag{11}$$

where $\boldsymbol{R_\varphi}$represents the stress terms, $\boldsymbol{M}_\varphi$, is the inter-phase momentum transfer terms and $\boldsymbol{S_u}$ represent various possible source terms.

The overall expressions $\boldsymbol{R_\varphi}$ and $\boldsymbol{M}_\varphi$ are split into several different terms which are user definable, and several different models exists for each of the different terms. The solver structure is generic in the sense that all the terms are evaluated and included, but in practice the user may leave out terms that are not applicable or relevant for the simulations. Thus, the same solver structure can in principle represent many different types of flow problems.

When simulating practical, industrial scale problems, usually the turbulent flow cannot be fully resolved and Reynolds Averaged Navier-Stokes (RANS) modelling is applied instead. To take into account the effects of the modelled turbulence, turbulence stress terms and turbulent dispersion models need to be activated to take into account the enhanced mixing due to unresolved fluctuations.

For two phases 1 and 2, the inter-phase momentum transfer in a turbulent flow would contain at least the following terms

$$\boldsymbol{M}_1 = K_d(\boldsymbol{U}_1 - \boldsymbol{U}_2) - \boldsymbol{M}_L - K_{vm}\left(\frac{D\boldsymbol{U}_1}{Dt} - \frac{D\boldsymbol{U}_2}{Dt}\right) - \boldsymbol{M}_{TD} - \boldsymbol{M}_{WL} \tag{12}$$

and

$$\boldsymbol{M}_2 = K_d(\boldsymbol{U}_2 - \boldsymbol{U}_1) + \boldsymbol{M}_L - K_{vm}\left(\frac{D\boldsymbol{U}_2}{Dt} - \frac{D\boldsymbol{U}_1}{Dt}\right) + \boldsymbol{M}_{TD} + \boldsymbol{M}_{WL} \tag{13}$$

where K_d and K_{vm} are momentum transfer coefficients for the drag and virtual mass forces. $\boldsymbol{M}_L$, $\boldsymbol{M}_{TD}$ and $\boldsymbol{M}_{WL}$ are force vectors due to lift, turbulent dispersion and wall lubrication forces.

In OpenFOAM, the turbulent dispersion term between the dispersed and continuous phases is written as

$$\boldsymbol{M}_{TD} = D_{TD}\nabla\left(\frac{\alpha_d}{\alpha_d + \alpha_c}\right) \tag{14}$$

where D_{TD} is a turbulent dispersion diffusion coefficient which is provided by a dispersion model. If the case consists of only two phases, the term further simplifies to

$$\boldsymbol{M}_{TD} = D_{TD}\nabla\alpha_d \tag{15}$$

From this expression it can be seen that the effect of turbulent dispersion is to smoothen out the gradients of volume fraction in the flow.

As an example of a turbulent dispersion model, one commonly applied model is given by Burns et al. (2004), which can be written for two-fluids as:

$$D_{TD} = \frac{3}{4}C_d Re_d \frac{\nu_c \nu_{t,c}}{\sigma_\alpha d_d^2}\rho_c \alpha_d \left(\frac{1}{\alpha_d} + \frac{1}{\alpha_c}\right) \tag{16}$$

This is also known as the Favre Averaged Drag (FAD) model and has been developed by ANSYS CFX employees. In Ansys Fluent, a similar term is called the “Interphase Turbulent Momentum Transfer” term or as the turbulent drag term and written as a part of the drag coupling.

4.2 Turbulent dispersion with population balances

In many industrial processes, the flow is both turbulent and polydisperse. Thus, in the simulation both the population balance modelling and turbulent dispersion modelling are important and need to be considered. However, this is the point where there is a bit of fundamental incompatibility between the overall flow equations and PBEs as they are currently implemented. As far as we know, this incompatibility is not specifically limited to OpenFOAM implementation, but is a more general issue which also exist in other CFD packages.

In the derivation of PBEs, such as equation (1), the velocity field is typically considered to represent fully resolved velocity. That is, the velocity field should represent all advection of the size groups and the concepts of turbulence and turbulent dispersion do not exist at this level. This is in direct conflict with the RANS simulation approach, where the velocity field only represents the average motion and does not include the turbulent fluctuations. Turbulent effects are usually included in PBEs, but they are only limited to the source terms of the equation such as breakup or agglomeration, but not to the transport terms.

Some effect of turbulent dispersion is visible in the convection term of PBEs. The phase velocity used in the PBEs is calculated from the momentum equations (11), where the turbulent dispersion term (14) is included. The problem with this is that the term is evaluated based on the overall gradient of the dispersed phase, while in reality the dispersion affects the transport of the dispersed phase at the size group level. The dispersion models, such as the model by Burns et al. (16), are functions of drag and volume fraction gradient. The drag force is strongly a function of diameter and thus for similar levels of overall turbulence, the smaller size fractions should disperse more readily than larger size fractions. Perhaps more significantly, the direction of dispersion should be calculated based on the gradient of the individual size groups which can differ significantly from the overall volume fraction of the dispersed phase as shown in Figure 2 and Figure 3.

To summarize, in the current OpenFOAM implementation of turbulent dispersion together with population balance there are at least the following issues:

1. Individual size groups do not see any effect of turbulent dispersion expect for the bulk term from the phase-level turbulent dispersion force (14). The phase-level dispersion force affects phase velocities, and this is visible in the convection term in PBEs. However, the correct level of dispersion of individual size groups could be very different from the level of the net dispersion.

2. The proper amount of net dispersion that a polydisperse phase encounters cannot be calculated based on the overall volume fraction and overall drag. If the net amount of dispersion is needed, separate contributions would need to be calculated for each size fraction and then these contributions could be summed.

3. The direction of dispersion is the same for all size groups, although in reality differently sized particles can disperse in opposite directions as the gradients of individual size fractions are not the same as the gradient of the overall volume fraction. For example, there might not be a volume fraction gradient in the overall phase fraction, but individual size groups can have gradients which should even out due to turbulent dispersion.

4. As the turbulent dispersion is calculated at the phase, i.e. velocity group level, the resulting amount and type of dispersion is strongly dependent on how many velocity groups are applied in the simulation. If turbulent dispersion is important for the flow problem, the simulation results become very sensitive to the choice of velocity group discretization. In the worst case to a point where this can determine the results.

When looking at this list of issues, one root cause is that with the velocity group concept we are stating that certain size groups share a common velocity. Yet from the dispersion point of view, we would still need the size groups within that velocity group to disperse with different rate depending on their size, which is a contradiction. A straightforward solution would be to create a separate velocity group for each size group and this approach would likely work and resolve the issues even with the current implementation. However, this is purely academical as such approach would be much too computationally prohibitive in any practical case. Some other, less computationally intensive solution is needed.

4.3 Numerical example of the issue with dispersion modelling

The issues with turbulent dispersion can be easily demonstrated by using a set-up illustrated in Figure 4. In the set-up, a distribution of $n = 20$ bubble size groups f_i is injected into a domain of size $L \times H$ from the bottom at $x = 0$. Initially, the domain is filled with liquid-gas mixture with $\alpha_l = 0.9433$ and a uniform distribution of bubbles of size d_0 moving towards the outlet ($x = H$) with velocity $U = 0.916$ in a turbulent $k > 0$, $\omega > 0$, $\nu_t > 0$ flow field. The inlet velocity and turbulence values are the same as the initial condition.

From a physical point of view, after some distance from the inlet, the turbulent fluctuations should mix the size groups resulting in a uniform spatial distribution of $f_i = 1/n$ at the outlet. However, it can be observed that using the models readily available in OpenFOAM, the bubbles do not mix and the same distribution, which is set at the inlet, flows through the outlet. The effect is illustrated in Figure 5.

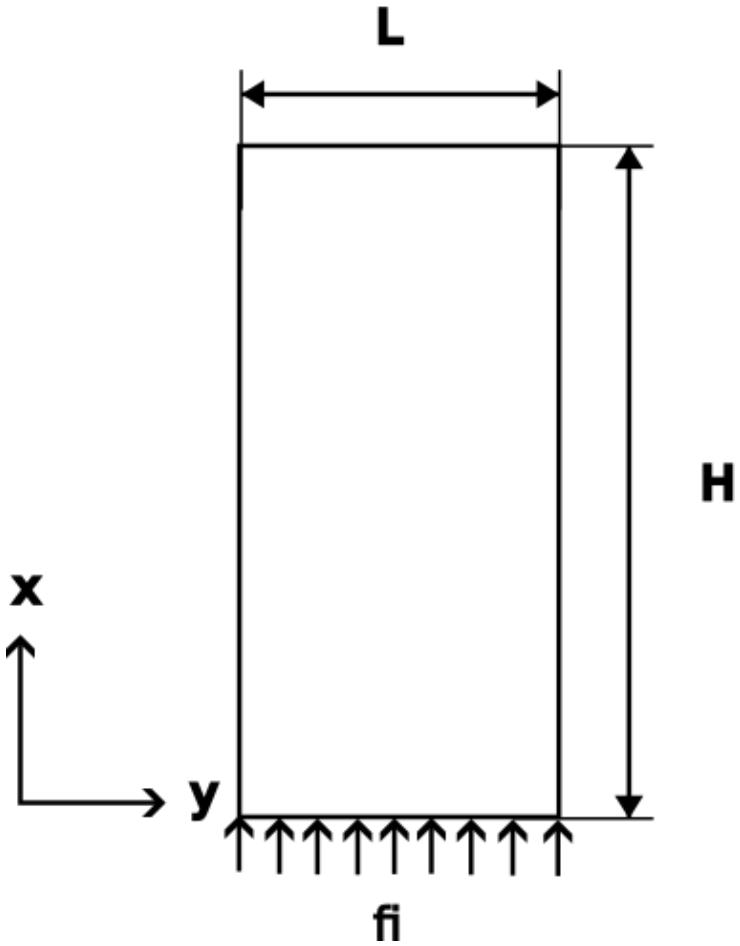

Figure 4. Sketch of the model problem setup.

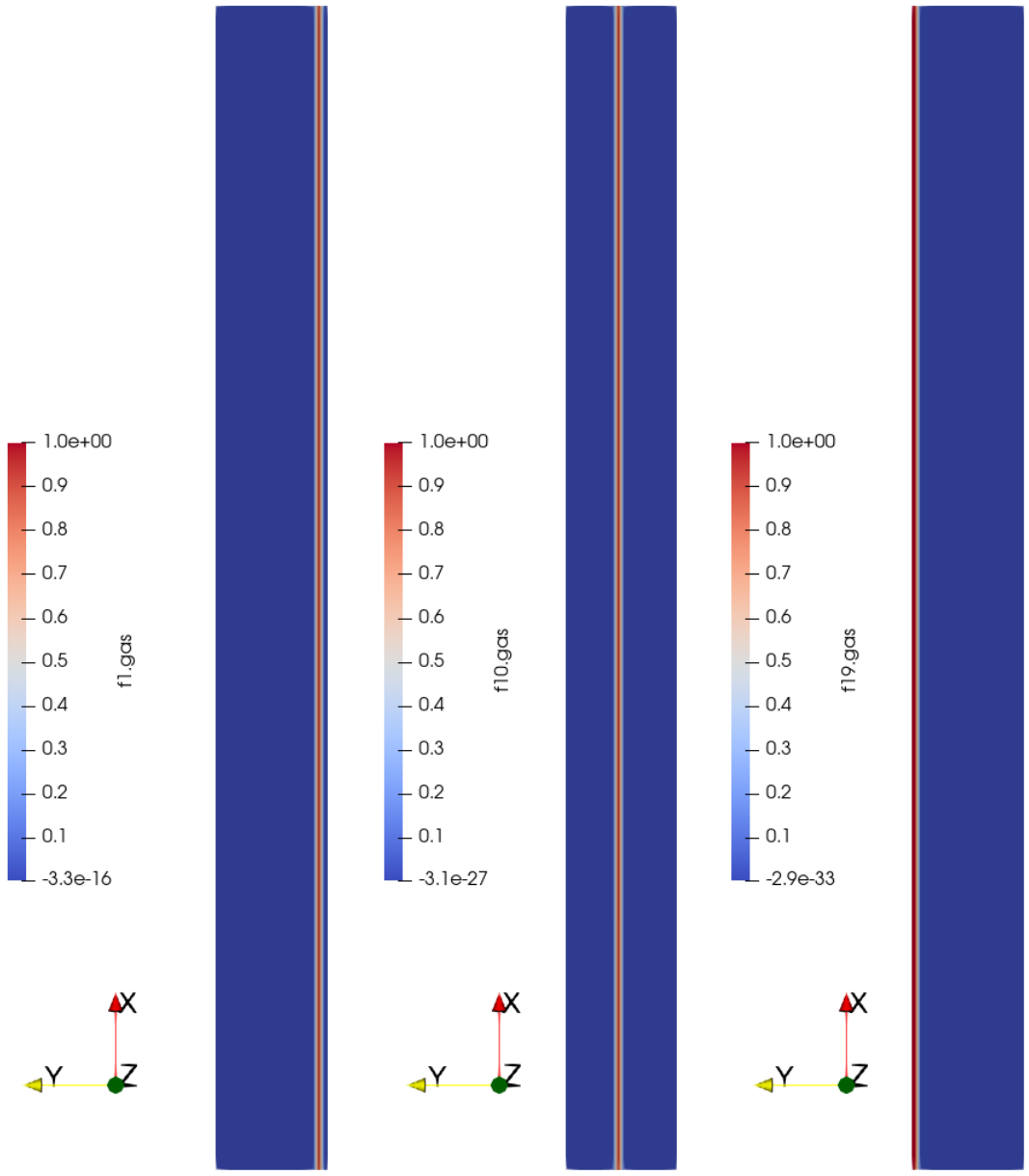

Figure 5. Illustration of size groups f_1, f_{10}, f_{19} not properly mixing in a turbulent flow field.

4.4 Discussion and proposed remedies for the dispersion modelling

Of the issues listed in section 4.2, the second issue could be solved in a relatively straightforward manner. As a first order approximation, instead of calculating a common dispersion term for the whole dispersed phase or velocity group, similar models can be used but just evaluated separately for each size group. The net dispersion would be obtained as a sum of the components

$$\boldsymbol{M}_{TD} = \sum_i D_{TD_i} \nabla \left(\frac{f_i \alpha_d}{f_i \alpha_d + \alpha_c} \right) \tag{17}$$

This change would require some modifications to the solver structure, and it would add some computational overhead, but the changes should be relatively unobtrusive and the performance impact modest.

When the turbulent diffusion is modified at the momentum equation level, the effect becomes visible to the PBEs through the velocity field in the convection term. However, as discussed in section 4.2, this alone does not allow different rates of dispersion for different size groups. With the convection term different size groups are all advected with the same flux based on their relative amounts. To rectify this, additional modification of the PBEs is needed.

In principle it would be easy to add additional terms to the PBEs to account for additional effects such as dispersion or the convection term could be modified to be size dependent. However, the key issue is that the solution of the size fractions should be compatible with the phase fraction field and satisfy the conditions given in (5). If additional terms are added to the PBEs, it is quite easy to end up violating these conditions. Even in the current implementation, which is formally valid and conservative, in practical simulations the size fractions often drift so that they do not sum up to unity. In practice what is done is that after solving the transport equations, the size fractions are scaled and limited so that the conditions (5) are satisfied. If this is not done, the simulations would drift into unphysical state.

This kind of scaling, when done in moderation, is usually not too problematic. However, it can also easily mask serious errors in the implementation or case setup, and it breaks the conservation of the size fractions. This can lead to results which are driven by numerical tricks instead of the actual physical models leading to wrong conclusions about the applicability or validity of the models. For this reason, both the mathematical formulation and the actual implementation should be such that minimal amount of scaling and compensation should be needed.

One possible option to solve the consistency issue would be to remove the phase fraction transport equations entirely and compute the overall dispersed phase fraction by summing the individual size group concentration fields. However, such refactoring would be a major undertaking as all the existing submodels and solvers follow a certain structure. It is also not clear how e.g. the pressure-velocity coupling should be modified to work in this kind of approach without resorting to the "separate velocity field for each size group" -approach.

The transport of the size fraction fields shares quite much analogy with the transport of chemical species. In multicomponent flows, for each chemical specie mass fraction Y_i, a transport equation is solved

$$\frac{\partial(\alpha_\varphi \rho_\varphi Y_i)}{\partial t} + \nabla \cdot (\alpha_\varphi \rho_\varphi \boldsymbol{U}_\varphi Y_i) + \nabla \cdot J_i = S \tag{18}$$

The mass fractions must satisfy the same conditions as size group fractions, i.e.

$$0 \leq Y_{i_i} \leq 1, \qquad \sum_i Y_i = 1 \tag{19}$$

This is very similar to the transport equation of size groups, but here the equation also contains an additional term $\nabla \cdot J$ which represents the diffusion of individual specie. A typical formulation is

$$J_i = -D_{eff,i} \nabla Y_i \tag{20}$$

where $D_{eff,i}$ can account for both laminar and turbulent diffusion. A diffusion term has many attractive features as it is conservative and it also has the correct form to represent dispersion, so it would be tempting to add such a term to the PBEs. However, the requirement of size fraction summing up to unity adds constraints on how this term can be formulated.

To use the specie equations as an example, in order not to create any overall net flux, the sum over all the components of the diffusion term must vanish.

$$\sum_i \nabla \cdot J_i = 0 \tag{21}$$

From the constraint

$$\sum_i Y_i = 1 \tag{22}$$

it follows that

$$\sum_i \nabla Y_i = 0 \tag{23}$$

and also

$$\sum_i \nabla \cdot D_i \nabla Y_i = 0 \tag{24}$$

but only if D_i is (locally) constant and the same for each term. If D_i is not constant, it would need to be carefully chosen in such a way that the sum would vanish. As the turbulent dispersion is a function of the particle size, ideally different size fractions should have different diffusion coefficients.

In older version of OpenFOAM, all species had a common diffusion coefficient which naturally satisfies the constraint (24). In newer versions of OpenFOAM non-uniform specie diffusion support was added for example by Fickian and MaxwellStefan binary diffusion models, which produce different diffusion terms for each specie. When this feature was implemented, it became mandatory to define a default specie which is not solved for but instead calculated as

$$Y_{default} = 1 - \sum_i Y_i \tag{25}$$

The default specie compensates the imbalance if the underlying diffusion models do not satisfy equation (25), which they usually don't. It also absorbs any numerical errors arising from the discretization, conservation, or source terms.

With chemical species selecting a default specie is frequently possible as there often is a relatively abundant background specie present. For example, nitrogen is a common choice when air is present in the system. But even with chemical species, there are cases where such a background specie does not exist. With PBEs a similar strategy could be followed, but for size fractions and especially with multiple velocity groups it is much less straightforward to determine which fraction would be suitable to be chosen as default. For this reason, the formulation of the diffusion term should be such that constraint (24) is satisfied as closely as possible.

As the turbulent dispersion is a function of the particle size, ideally different size fractions should also have different diffusion coefficients similarly to non-uniform specie diffusion. However, because it is not easy to determine a default size group, the diffusion coefficients should be chosen so that the individual diffusion fluxes of the size groups would balance each other. At present it is unclear what would be the best way to achieve this and further investigation would be needed.

As a simple starting point, however, and to still be an improvement compared to the present situation, it would be possible to apply the approach (17) to determine the overall level of turbulent dispersion and add a diffusion term to PBEs with a common diffusion coefficient.

4.5 Preliminary numerical tests with per size class dispersion

To test how the proposed solution strategy would work, several numerical test simulations were performed where an additional diffusion term $\nabla \cdot \left(\alpha_\varphi D_k \nabla f_i\right)$ was added on the RHS of the PBEs resulting in equations of the form

$$\frac{\partial \alpha_d f_i}{\partial t} + \nabla \cdot (\alpha_d \boldsymbol{U}_d f_i) = \nabla \cdot \left(\alpha_\varphi D_k \nabla f_i\right) + S_{ij} \tag{26}$$

where D_k is a diffusion coefficient. In a similar test as in section 4.3, the effect of the added diffusion term is clearly visible. In Figure 6 an example is given for $D_k = 0.0001$. As can be seen from the figure, the additional diffusion term produces a physically reasonable solution where size groups disperse evenly in the whole domain cross section along the flow direction.

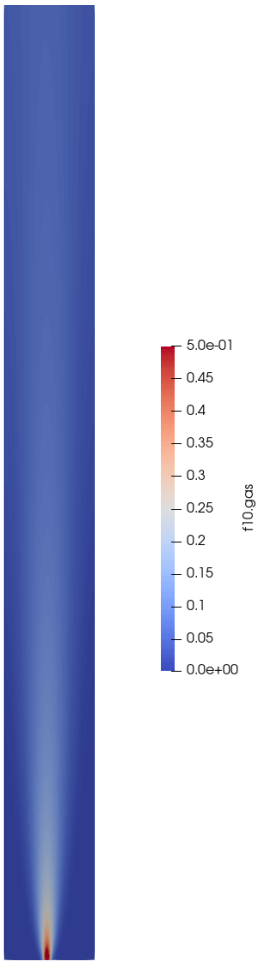

Figure 6. The effect of adding a diffusion term to the population balance transport equation.

In addition to testing with a single velocity group, tests were performed with two velocity groups. An example of such test is shown in Figure 7. In this case the injected gas is split into two velocity groups with the same properties. The first 10 bubble size groups are assigned into gas1 and the remaining 10 into gas2. As can be seen from the figure, gas2 is injected from the left side of the inlet and the size group f_{11} is initially within gas2. With the added diffusion term, the size fractions disperse within their respective velocity groups. There is no mixing between the velocity groups, since turbulent dispersion between the velocity groups was disabled.

From Figure 7 it can be also observed that with the inclusion of the diffusion term, the size fractions can start to diffuse out of the region occipied by the velocity group. In purely mathematical form, diffusion term should vanish in regions where phase fraction goes to zero. However, when the term is evaluated at the faces of the mesh, the volume fraction is typically linearly interpolated and remains finite.

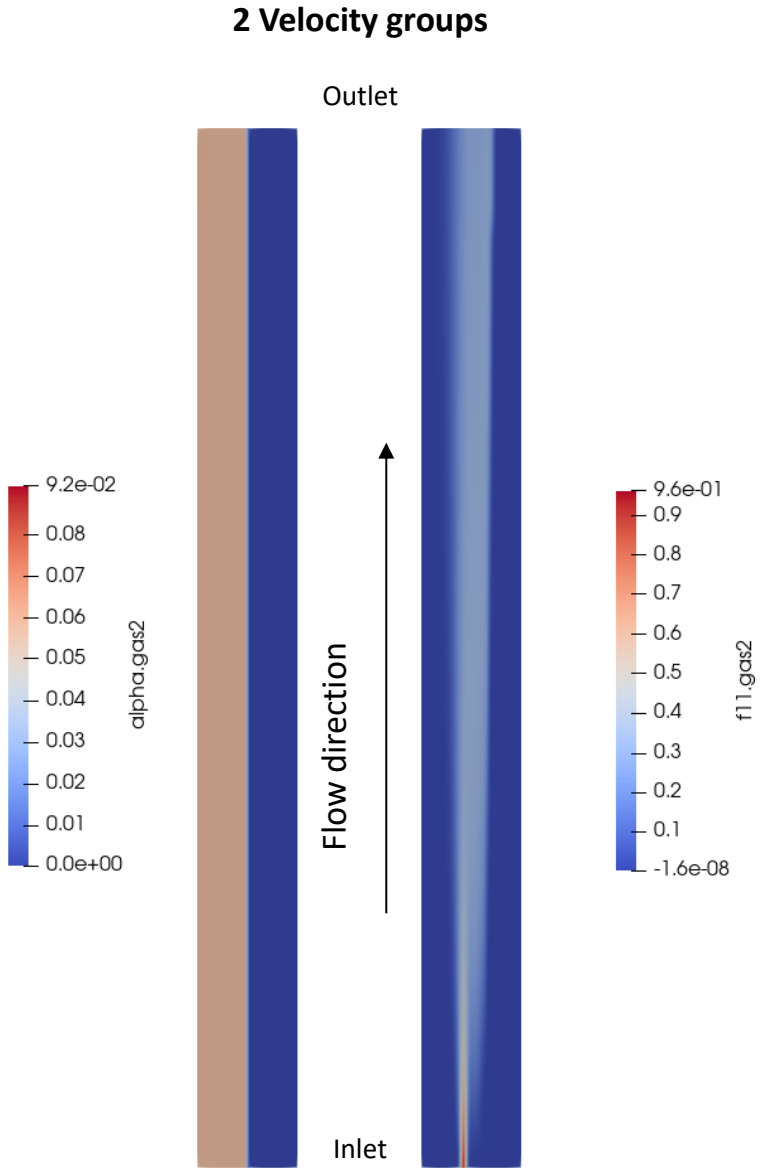

Figure 7. The result of the test case when two gasses are injected from the inlet at bottom. The figure shows the volume fraction of gas2 and the size group fraction f_{11} of that phase.

Although the addition of the diffusion term can cause the size fraction fields to diffuse out of the phase, based on the preliminary tests, volume concentrations of the individual size groups are still conserved. As an example, surface integrals of f_9 and $\alpha_d f_9$ over the inlet and outlet patch as a function of time are plotted in Figure 8. As can be seen from the figure, although the value f_9 increases due to diffusion, volume concentration $\alpha_9 = \alpha_d f_9$ is conserved between inlet and outlet.

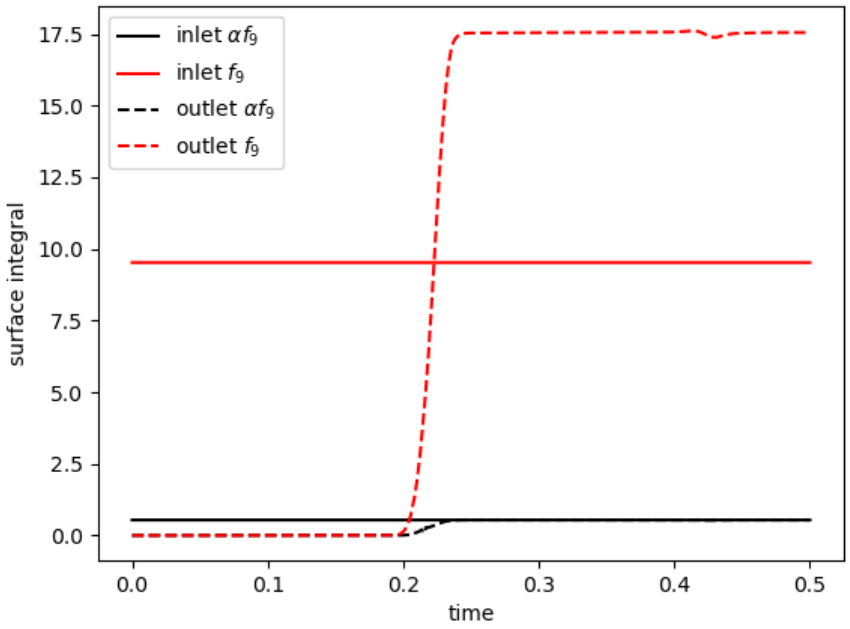

Figure 8. The flow rates f_9 and $\alpha_d f_9$ integrated over inlet and outlet as a function of time.

Based on the performed numerical tests, the addition of a diffusion term to the PBEs appears to be a relatively robust way to produce dispersion within the velocity groups, which is missing from the current implementation. However, at this point the results are only qualitative and further work would be needed to determine which way the diffusion coefficients should be calculated to produce quantitatively correct amount of dispersion. It should be also investigated if there is a method to evaluate non-uniform diffusion coefficients but still reliably satisfy constraint (24).

5. Summary and conclusions

In the present report, we have demonstrated that the current OpenFOAM class method population balance model is incapable of properly taking into account the effect of modelled turbulence in the dispersion of bubbles or particles in turbulent polydisperse multiphase simulations. Proper treatment of turbulent dispersion is needed, because in many industrially relevant polydisperse flows turbulent mixing is an important feature of the flow. When using RANS modelling approach, a large fraction of turbulence is not directly resolved, and the effect of turbulent mixing needs accounted for in the closure models.

We note that similar problems also exist in other CFD packages, so the deficiencies presented are more general issue on how the turbulent dispersion is modelled with polydisperse flows. Resolving the issues in numerically robust and efficient ways is not completely straightforward. Various ways how to tackle the issues are discussed. However, we propose here an alternative formulation of the transport equation of the bubble size groups with an extra diffusion term added. Preliminary tests with the alternative formulation appear promising and qualitatively correct, but further work is needed to obtain a practical implementation which can produce also quantitatively good results.

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