

Numerical and Experimental Studies on PBEs in OpenFOAM Environment

Evren Bayraktar*

Institute of Applied Mathematics (LS III), TU Dortmund
Vogelpothsweg 87, D-44227, Dortmund, Germany.

E-mail: `Evren.Bayraktar@mathematik.tu-dortmund.de`

Abstract

The population balance model which was developed and verified in the FEATFLOW environment has been implemented into OpenFOAM software package. Sulzer CompaxTM mixer is numerically studied with the developed computational tool. The numerical results have been compared with experimental ones and the results have been found to be in good agreement. An interesting experimental finding, decreasing Sauter mean diameter of the droplet ensembles with increasing holdup of the secondary phase, has been investigated and explained with the population balance model coupled CFD simulations in 3D.

1. Introduction

Solutions and implementations of population balance equation coupled to turbulent fluid dynamics have been issued in detail in the previous reports and studies [1, 2]. The verified implementation of population balance model in the FEATFLOW environment is carried into the OpenFOAM environment with this study.

The population balance model is implemented in a stationary one-way coupled strategy in the OpenFOAM environment. The effect of dispersed phase on the flow is neglected and the population balance equations are calculated for a quasi-stationary flow field, for the details of implementation and the considered couplings reader is referred to [1].

The PBEs library, popBal, which was written in Fortran 90 programming language was coupled to OpenFOAM via a C programming language interface. Then, a customized application, nScalarTransportFoam, based on the standard application scalarTransportFoam is created. Later, this customized application is coupled with popBal to achieve the desired realization of stationary one-way coupled PBE-CFD application.

In this report, the developed computational tool is used to numerically study Sulzer static mixer, CompaxTM. Obtained numerical results are compared with the available experimental results for a certain volumetric flow rate and a range of holdup values. The agreement of experimental and numerical results found to be satisfactory.

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2. CFD Results

The geometry of the computational domain is provided by Dr. Hirschberg from Sulzer Chemtech in Stereolithography Interface format. The provided geometry file describes the flaps of CompaxTM mixer (dn20) and the pipe. The provided pipe geometry was unnecessarily long for the calculation of PBEs. Therefore, the STL file was modified in a way that the static mixer inserted pipe is 19 cm long.

The new geometry was meshed by using the snappyHexMesh pre-processing tool with two different set of parameters in order to have one fine mesh on which CFD simulations are performed to obtain a quasi-stationary flow field, and one coarse mesh on which PBEs are calculated by using the interpolated results of the CFD simulations. The fine and coarse meshes have 2,115,098 and 314,522 cells respectively. In Figure 1, the snapshot of cross sectional meshes are presented in and behind the mixer region where the mesh density is the highest.

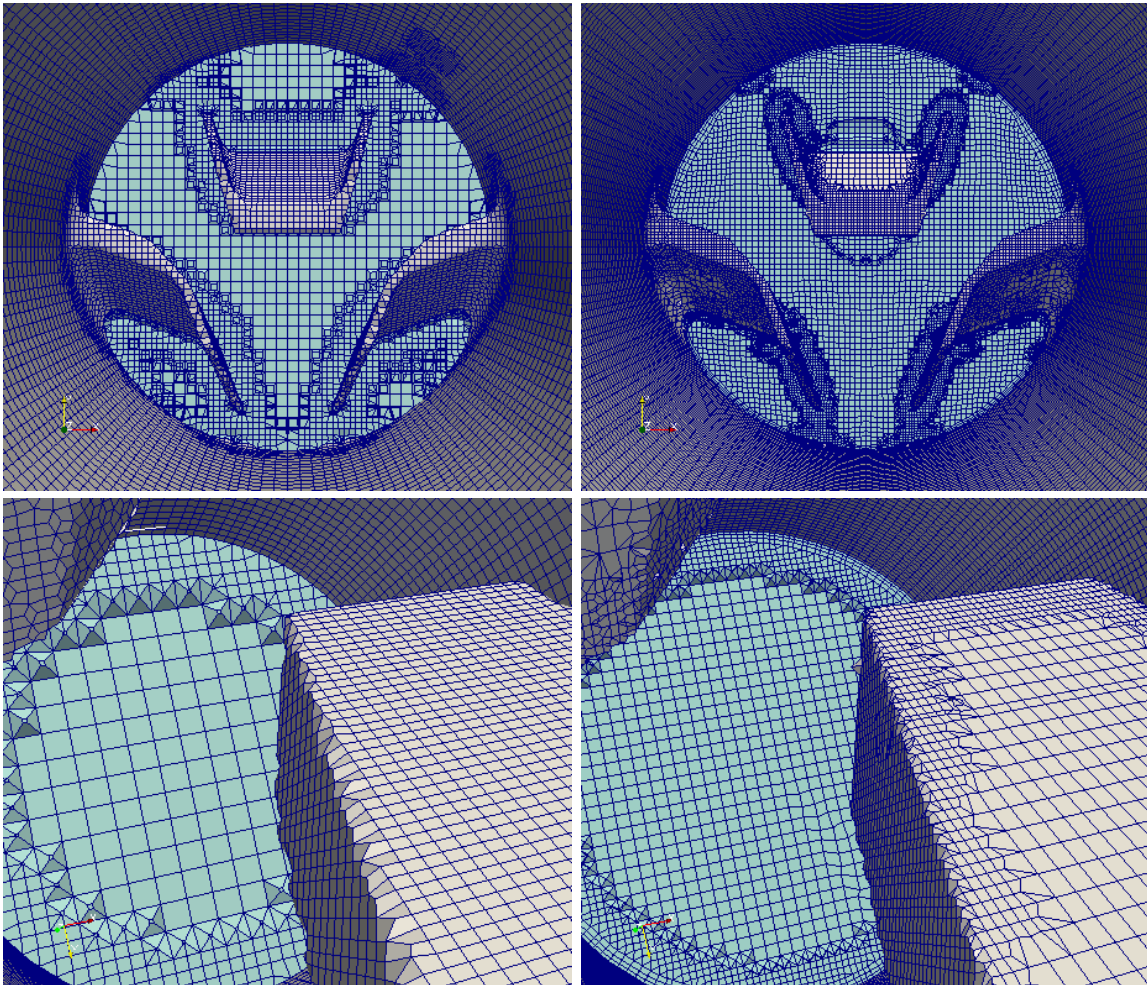


Figure 1: Snapshots of the mesh in and behind the mixer region; left: coarse, right: fine. The solid and fluid domains have grey and blue colors respectively.

The main differences in the presented meshes are the fine mesh has a nice boundary layer of 3 cells which increases the accuracy of the turbulent flow simulations and the local cell

size is approximately half of the coarse one.

OpenFOAM offers several applications customized for problems described with certain physics. The simpleFoam application which is a steady solver for laminar and turbulent flows was chosen for our purposes. $k-\varepsilon$ two-equation model which falls into category of Reynolds Averaged Navier-Stokes models has been chosen from the available turbulent models. First, the quasi-stationary flow field is obtained on the fine mesh and the results are interpolated onto coarse mesh by using mapFields utility of OpenFOAM. Snapshots of the calculated and interpolated CFD results are presented in Figure 2 and Figure 3 for the inflow velocity of 1m/s .

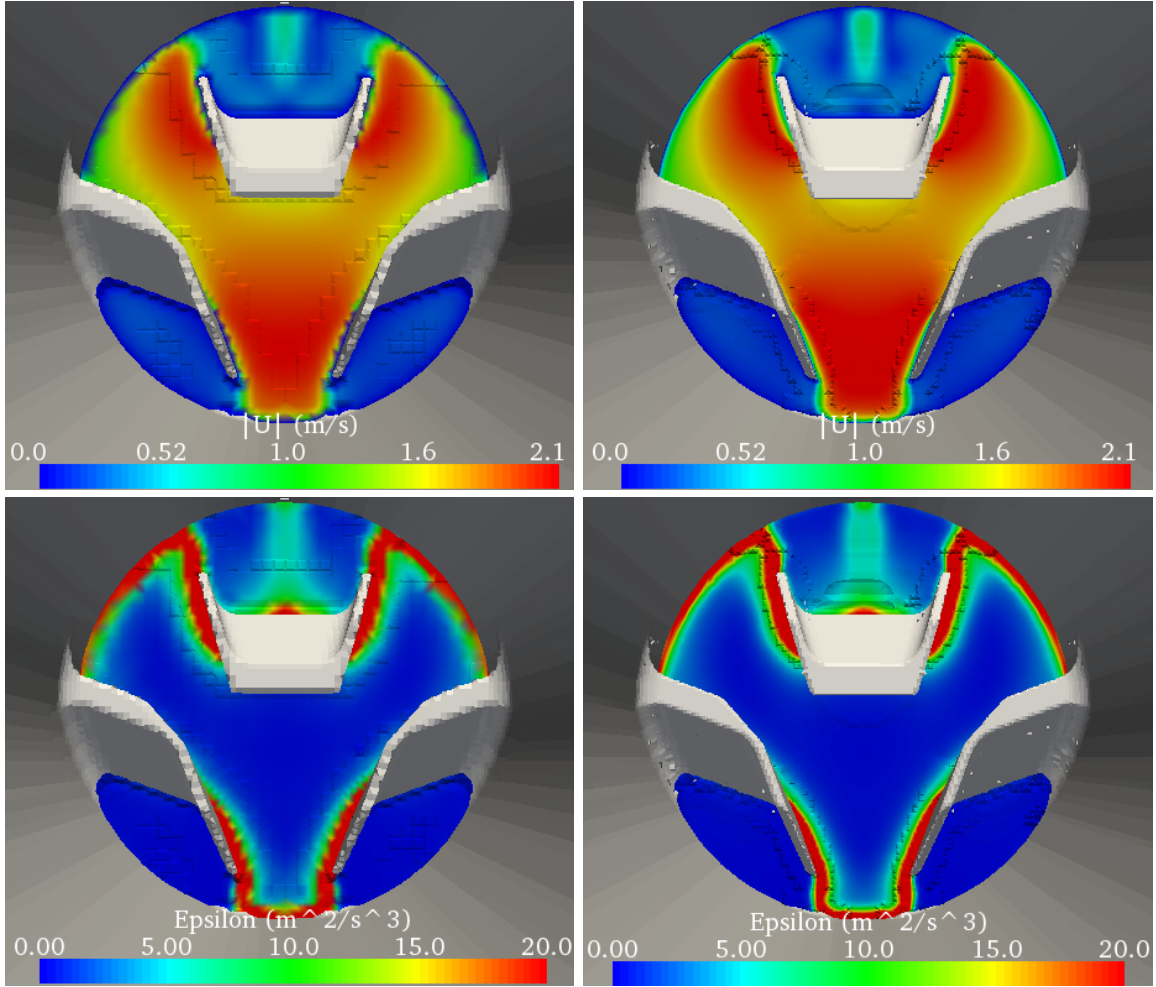


Figure 2: Snapshots of the interpolated and calculated CFD results in the mixer region, left and right respectively.

The presented results in Figures 2–4 show that both the calculated and interpolated results exhibit smooth profiles of the variables which are of interest. The results of the CFD simulation and the interpolation agree satisfactorily good to calculate PBEs.

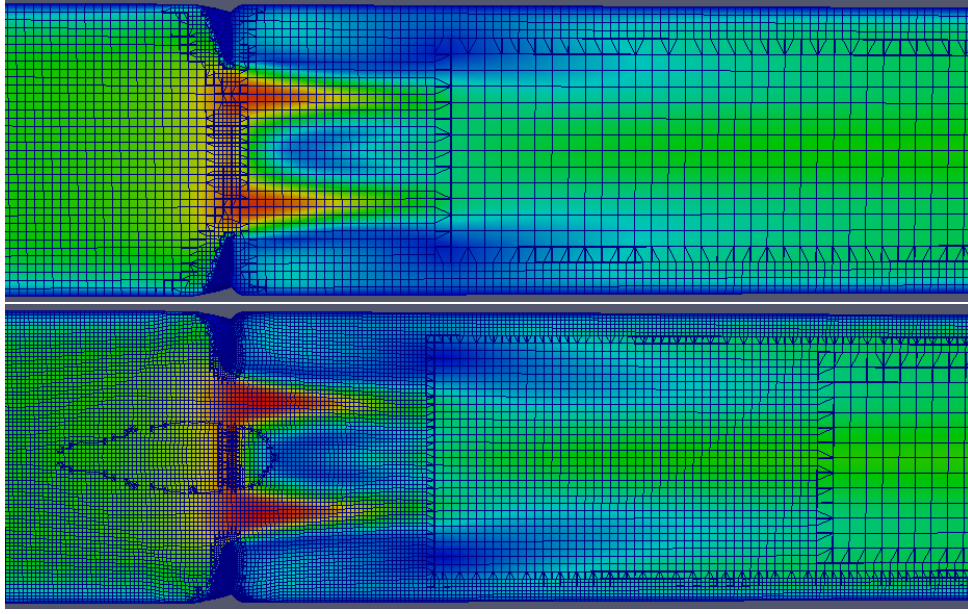


Figure 3: Snapshots of the interpolated and calculated results for the velocity magnitudes at the XY-Plane centered in the pipe, coarse and fine meshes respectively.

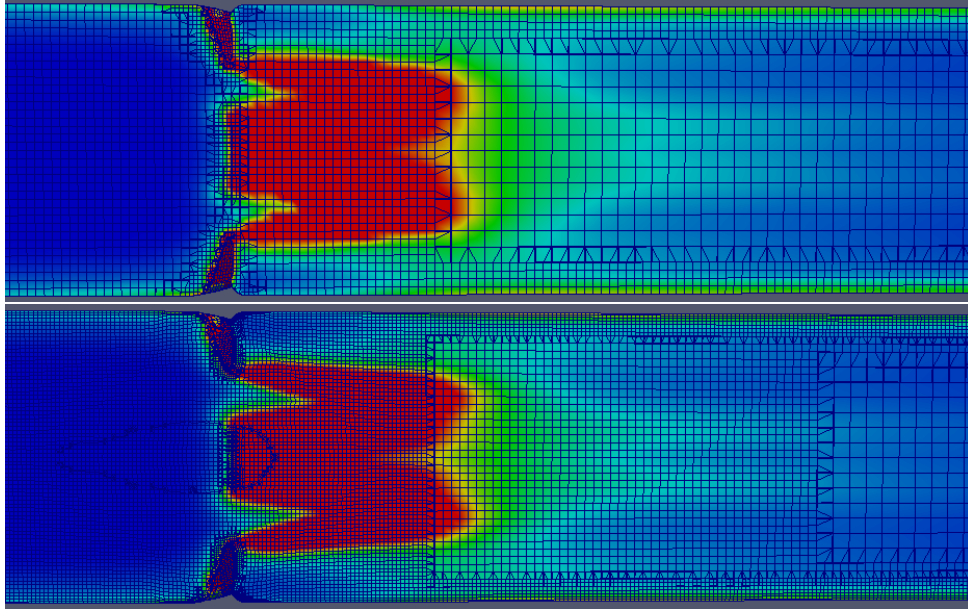


Figure 4: Snapshots of the interpolated and calculated results for the turbulent dissipation rates at the XY-Plane centered in the pipe, coarse and fine meshes respectively.

3. PBE Results

Accurate CFD results are the first prerequisite for the calculation of PBEs. The obtained coarse mesh and the interpolated CFD results can represent the geometry and the flow field sufficiently good while keeping the computational time and cost in reasonable range. The PBEs are solved by using the developed computational tool in the OpenFOAM environment for the obtained quassi-stationary flow field.

The PBEs are solved on the calculated flow field for four different holdup values: 10%, 15%, 20% and 25%. The physical parameters of the oil in water dispersion are as follows,

- density of water, $\rho_w = 1000 \text{ kg m}^{-3}$;
- density of oil, $\rho_o = 847 \text{ kg m}^{-3}$;
- viscosity of water, $\mu_w = 1 \text{ mPa s}$;
- viscosity of oil, $\mu_o = 32 \text{ mPa s}$;
- interfacial tension, $\sigma_{wo} = 0.043 \text{ N m}^{-1}$.

As the holdup values increase, accurate predictions to the experimental results get more challenging. The main reasons are the single phase approximation of the dispersion to simulate the flow field gets weaker and the PB model performs poorer for large fractions of the secondary phase.

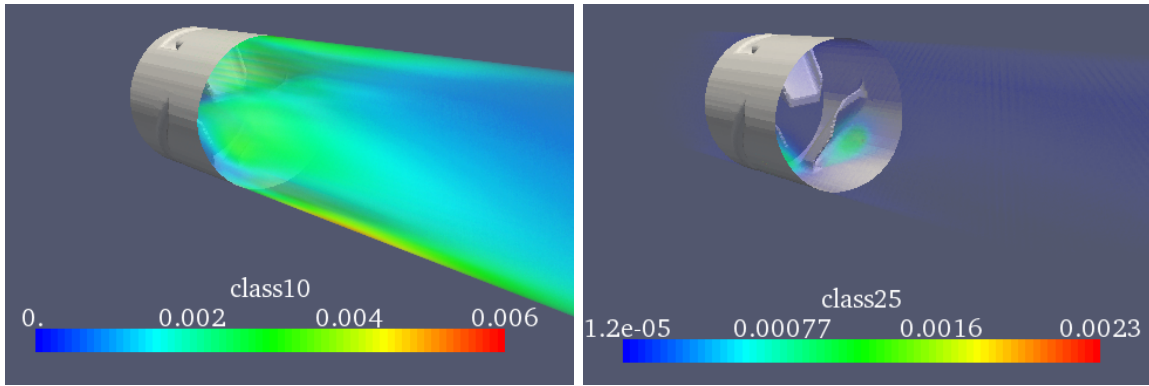


Figure 5: Holdup values of 15th and 25th classes.

Figure 5 and Figure 6 are given in order to give an insight to results of numerical simulations. In these figures, we see that a significant fraction of the initially introduced droplets (classes 15, 19, 23 corresponding to 0.58, 1.00 and 1.71 mm) still exists after the mixer region. This can have two explanations: the mixing is not very strong and only certain fraction of the droplets are coalescing and braking up, or the initial droplet size is close to the average droplet size at the equilibrium. This is very important for the numerical simulations because this implies that final results depends on the initial sizes.

To investigate this result, two calculations with different initial conditions are done. In these cases initial droplet sizes are set to 1 mm and 2 mm. In Figure 6 it is visible that regardless of the initial size of the droplets, the class which the droplets are initially set to has a significant and much larger holdup values than the other classes.

To see the influence of the initial size on the droplet distribution behind the static mixer, a volume averaged Sauter mean diameter (d_{32}) and volume averaged droplet size

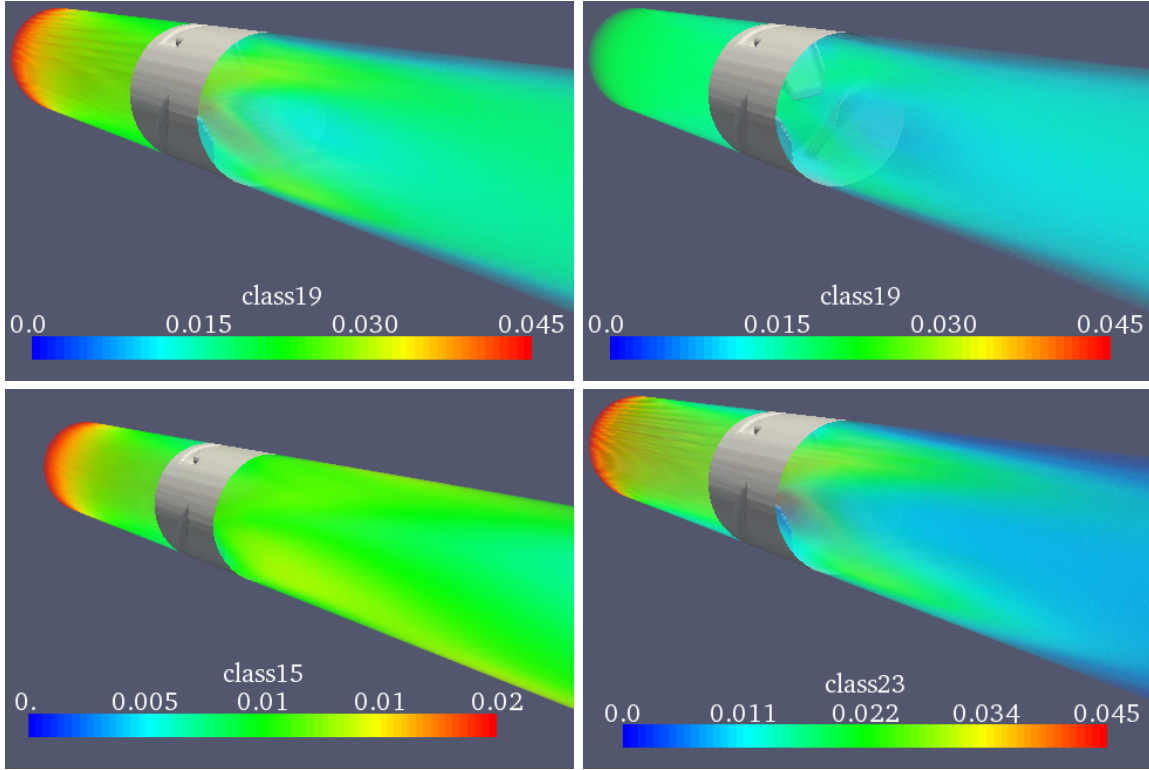


Figure 6: Top: Initial droplet size is 1.00 mm with different holdup values. Bottom: Initial droplet sizes are 0.58 mm and 1.71 mm

distribution is calculated at the cross section, $z = 0.12m$ and the results are presented in Figure 7. These results are sufficient to conclude that the initial droplet size has a strong influence on droplet size distribution behind the static mixer and without knowing the initial size it is not possible to truly predict the experimental results.

The experimental results are obtained by processing the pictures taken through the experiments. The experimental setup, measurement techniques, and evaluation of experimental data were explained in detail in the previous report and it is assumed that they are well known to co-workers at Sulzer Chemtech; therefore, they are not reconsidered in this report which issues mainly the developed computational tool to solve PBEs in OpenFOAM environment.

In the preliminary numerical simulations, it is shown that one has to know the initial droplet size to accurately predict the experimental results; however, this information was not available. Therefore, first the experimental results are evaluated and the measured droplet size distributions and d_{32} are obtained, the results are given in Figure 8.

When the experimental results (Figure 8) are considered, interesting findings are revealed. One of the very obvious one, the change of d_{32} is in a very narrow range and the trend contradicts to the expectation. The second finding is the measured largest droplet size gets smaller as the secondary phase fraction increases, which is also a contradiction to our knowledge. However, in numerical simulations we have seen that a significant fraction

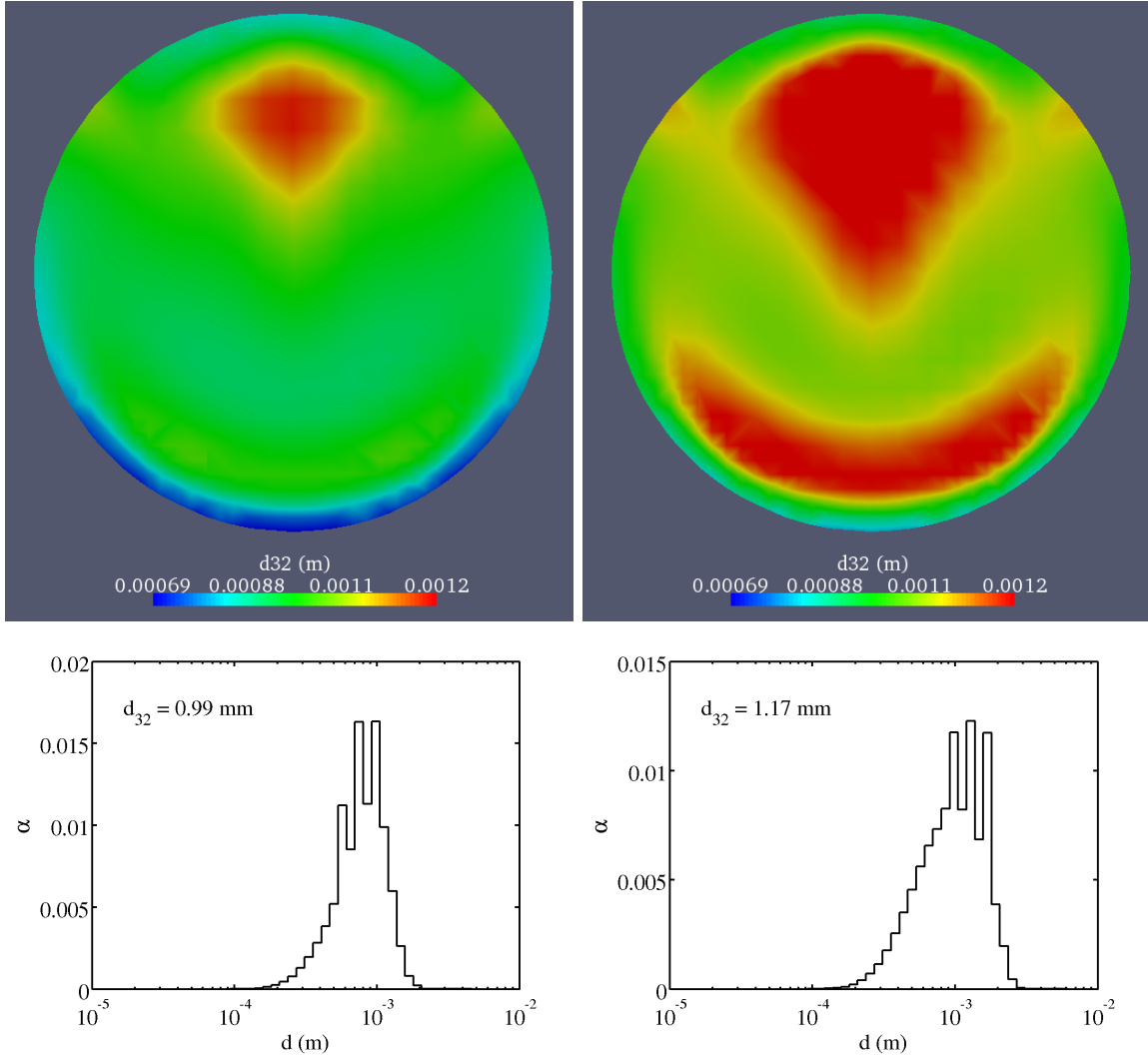


Figure 7: Sauter mean diameter and holdup distributions at the cross section $z = 0.12m$.

of the initial droplets, approximately 30%, still exists behind the static mixer and this is exactly what happens in the experiments, as well. As the secondary phase fraction is increased larger amount of oil flows into the pipe from the same inlet; therefore, the initial droplet size decreases with increasing the volumetric flow rate, fraction of secondary phase. This is supported by the finding: highest peaks in the graphs travel from right to left on the size coordinate as the holdup increases.

By judging on the experimental results (Figure 8), it is possible to determine the initial sizes or classes for the numerical simulation of the experiments. From Figure 8, the initial classes are determined as 29, 28, 27 and 26 (3.86, 2.94, 3.37 and 2.57 mm) for the holdup values of 10%, 15%, 20% and 25%, respectively. The numerical simulation of the experiments are done with these determined initial classes. In Figure 8, it is clear that the adopted discrete size coordinate in numerical simulations is sufficiently wide, however it is too fine to evaluate the experimental results. Thus, both experimental and numerical results are mapped onto a coarser grid for comparisons. In simulations, the discrete size coordinate is determined with the minimum size $v_{min} = 87 \times 10^{-6}$, discretization constant

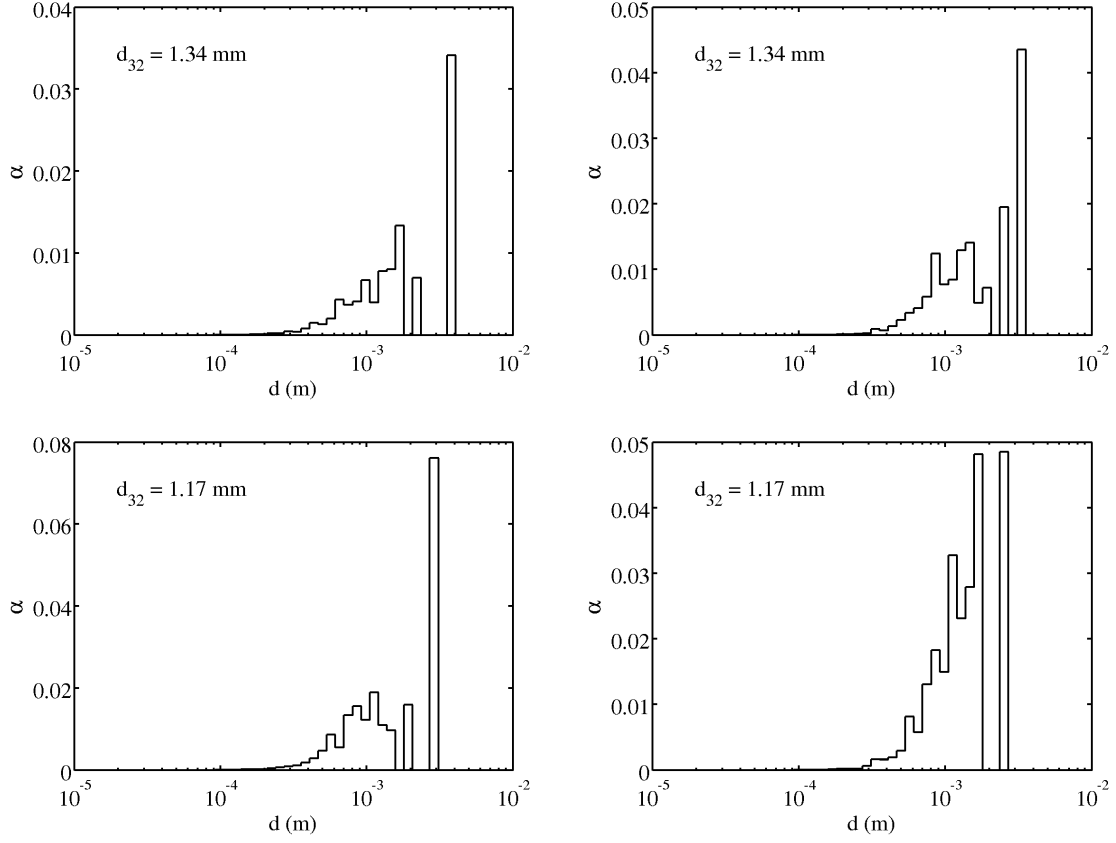


Figure 8: Experimental results.

$q = 1.5$, and 33 classes, the coarse size coordinate to compare the experimental and numerical results covers the same range with 21 classes.

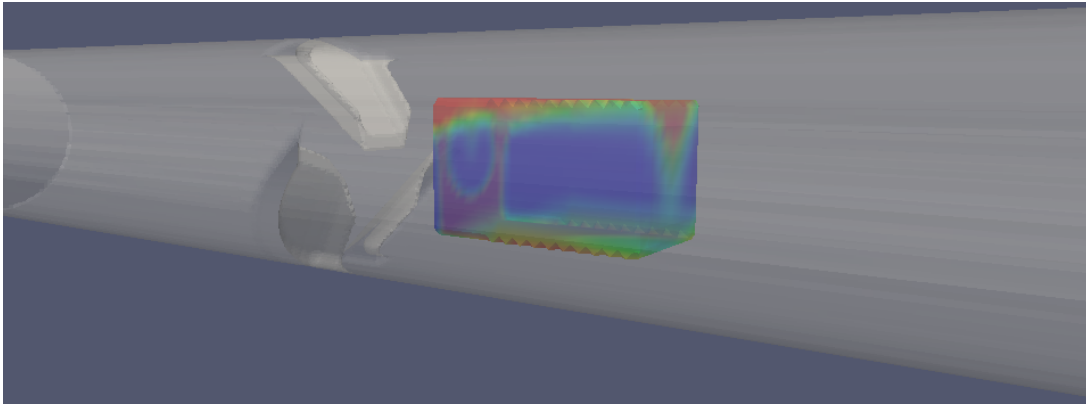


Figure 9: Control volume, $\Omega = (-0.006, 0.006) \times (-0.006, 0.006) \times (0.0805, 0.105)$.

It was shown that the size distribution across the cross section is not homogeneous, Figure 7. Therefore, a control volume which is similar to the pictured volume through the experiments is chosen right behind the static mixer, Figure 9. Then, the holdup of classes and Sauter mean diameters are integrated and are averaged within this control volume.

Later, the obtained results are mapped onto the coarse grid to have a better visualization of the numerical and experimental results, Figure 10.

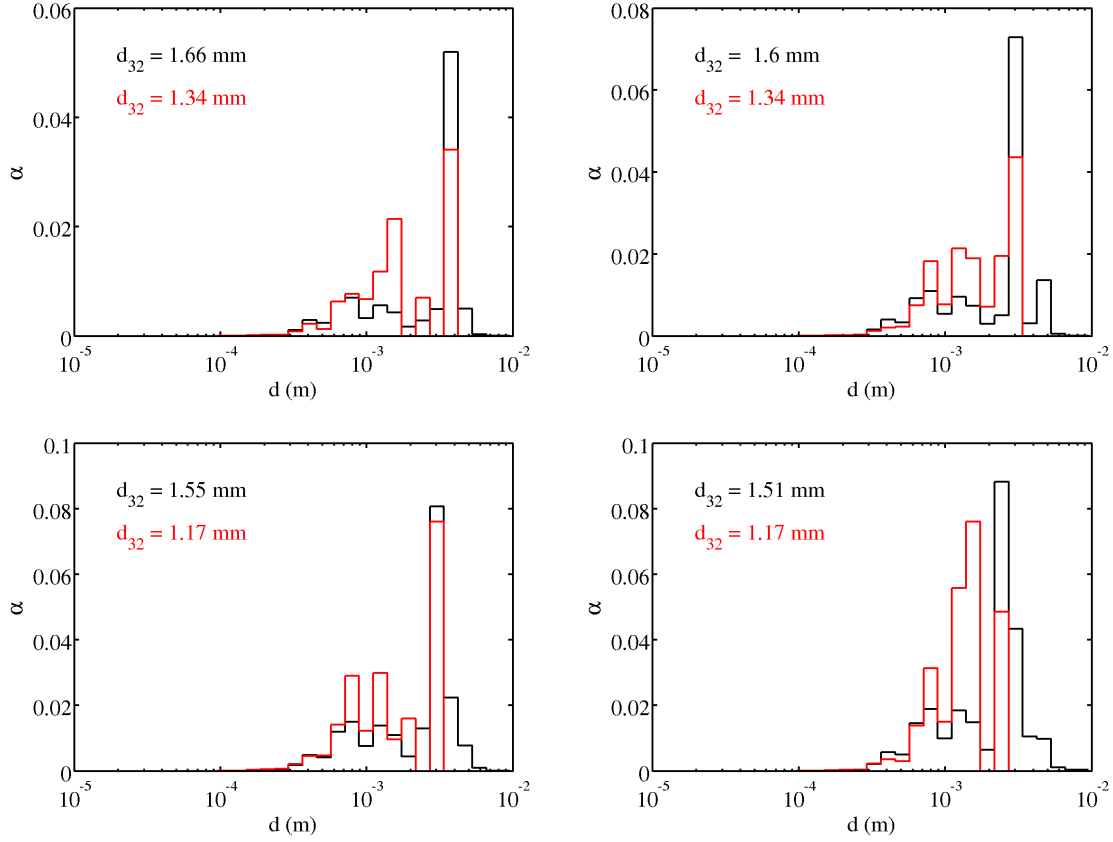


Figure 10: Comparison of experimental and numerical results.

Figure 10 presents that the experimental and numerical results are in sufficiently good agreement. The droplet size distribution and d_{32} have been predicted in reasonable ranges with the developed computational tool. The d_{32} values have about 20% differences which are acceptable for these type of problems. Moreover, sizes of the smallest droplets and the discrete droplet size distributions are predicted accurately. The numerical results are larger than the experimental ones. This was one of the conclusions that we had also in the previous study which was on the Sulzer SMVTM static mixers. Figure 10 leads to conclude that the adopted model results in high coalescence rates for large droplets even though, the coalescence kernel is modified with an additional term in order to yield lower coalescence rates for large droplets. However, it should be remarked that the large droplets are few in number but has a strong contribution to size distribution for holdup values. In the experiments, it is possible that these large droplets are not pictured; additionally, the introduced droplets assumed to be mono-dispersed which is not completely right: the dominant size is clear in the results but a certain fraction of the droplets can have significantly different sizes. Therefore, it is concluded that the actual size distribution is in between the measured and the calculated ones.

The second remarkable conclusion is that in both experimental and numerical studies Sauter mean diameter values are found to be decreasing with the increasing hold up values, 10. It is already said that being the initial sizes different is an explanation to this finding for the experiments; however, to see the same effect in the results of numerical simulations even for these small changes of values shows that the developed computational tool is sensitive to changes in operating conditions and is precise in the predictions. To investigate this finding further, the Sauter mean diameter values through the axis are plotted, Figure 11.

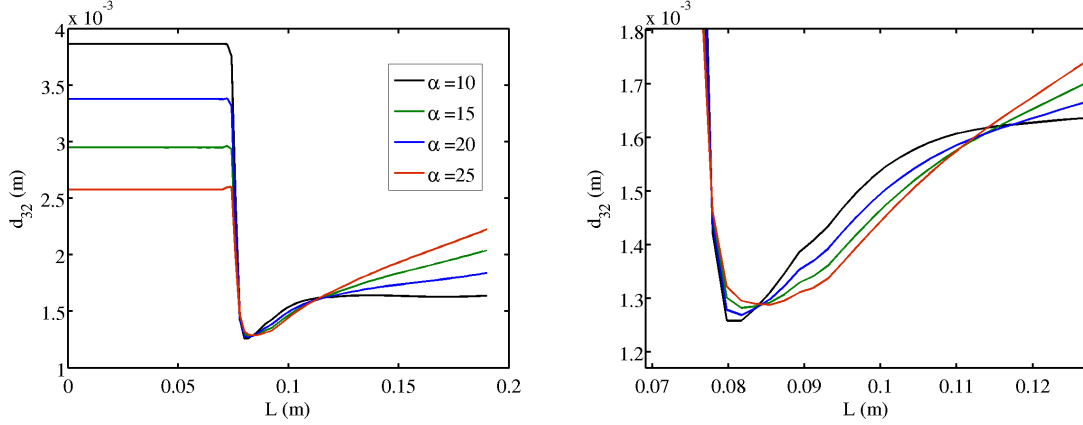


Figure 11: Sauter mean diameter through the pipe axis.

In Figure 11, it is visible that the second conclusion holds in a certain part of the pipe: $z = (0.07, 0.12)$. In this region, the d_{32} values change from 1.25 mm to 1.65 mm. Considering these values, it can be concluded that if the control volume was chosen somewhere else, the results would have better or worse agreement depending on location and size of the control volume. However, it should be mentioned that the control volume is chosen fairly far from mixer and reasonably large such that the volume averaging will give almost location independent results; yet, Figure 11 shows that droplet sizes change very rapidly in the measurement region.

4. Conclusion

Sulzer CompaxTM static mixer is numerically studied with the developed computational tool, population balance model coupled customized CFD solver in OpenFOAM environment. The numerical and experimental results are compared in detail and the interesting findings could be elucidated with 3D numerical simulations. The agreement of the results found to be satisfactory and the reasons of the discrepancies between experimental and numerical results are discussed. Consequently, it is shown that the developed computational tool can be reliably used to accurately simulate dispersed phase systems in complex geometries like static mixers.

References

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