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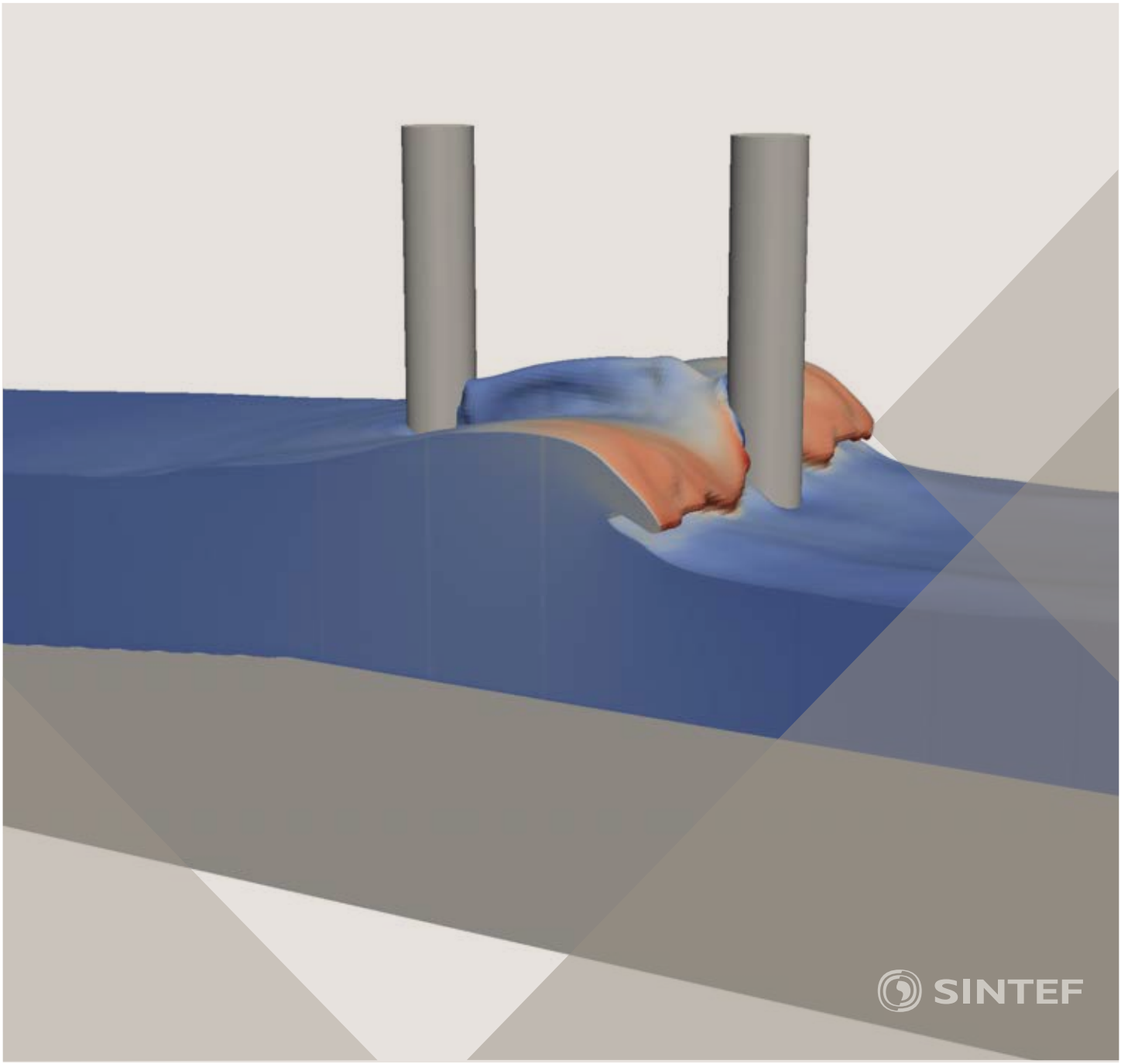

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Editors:
Jan Erik Olsen and Stein Tore Johansen

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

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CONTENTS

CFD SIMULATION OF THE DROPLET SIZE DISTRIBUTION OF LIQUID-LIQUID EMULSIONS IN STIRRED TANK REACTORS

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ABSTRACT

Predicting the drop size distribution (DSD) is essential in particulate flows such as emulsions as it affects mass transfer and heat transfer. In the current work we developed a novel numerical method to account for droplet breakup. The droplet breakup relies on an in-house developed correlation which depends on the local shear rate and some fluid properties. Commonly, a population balance equation (PBE) is employed to describe the breakup and coalescence of the droplets; however, such an approach does commonly not distinguish between different slip velocities of the smaller and larger droplets. Therefore, we propose a hybrid modelling strategy, which combines an Eulerian-Eulerian two-fluid model (TFM) and a Lagrangian discrete particle model (DPM), which is referred to as the Hybrid TFM-DPM model. This method enables the efficient evaluation of the poly-disperse liquid-liquid drag force form the local distribution of the different droplet diameters. The latter can be obtained by tracking statistically representative droplet trajectories for each droplet diameter class. Finally, we applied this novel approach to a liquid-liquid emulsion in a stirred tank presented. The results clearly show that the present method is able to predict the droplet size distribution for different rotational speeds of the stirrer.

Keywords: Emulsion, Droplet breakup, Coalescence, Hybrid TFM-DPM

NOMENCLATURE

Notation

We Weber number, [-].

Re Reynolds number, [-].

A Dimensionless constant, [-].

a Shear rate, [-].

D_{32} Sauter mean diameter, [m].

D_{90} 90% of the droplets are smaller than this value, [m].

F_k^{poly} Drag force acting on a parcel with d_k ,[kg. m/s^2].

g Gravity acceleration, [m/s^2].

h Characteristic length, [m].

K Interphase momentum exchange coefficient

L Impeller diameter of stirred tank (Characteristic length), [m].

$\vec{u}$ Velocity field, [m/s].

$\widetilde{u}$ Average velocity, [m/s].

Greek Symbols

ρ Mass density, [kg/m^3].

μ Dynamic viscosity, [kg/m.s].

γ Interfacial tension, [kg/s^2].

ε Turbulence dissipation rate. [m^2/s^3].

ς Collision frequency, [#/s].

λ Coalescence efficiency, [-].

Γ Coalescence frequency, [#/s].

τ Shear stress, [kg/m.s^2].

$\tau_{col.d}$ Collisional time scale.

ϕ Dispersed phase volume fraction. [-]

Sub/superscripts

c Continuous phase.

d Dispersed phase.

k Index of parcel.

p Parcel.

INTRODUCTION

Emulsions are widely used in the several industries such as food, pharmaceutical, cosmetic, chemical and petroleum. Drop size distribution (DSD) plays the key role as it controls mass transfer and heat transfer of the liquid-liquid system inside the reactor (Leng and Calabrese, 2004). Wide range of studies are done both numerically and experimentally to cover the DSD issues in the stirred tank reactor. There are several experimental studies focus on the single drop breakup experiment in order to define the breakup kernel for the Population balance equation (PBE) (Maaß et al., 2012; Solsvik et al., 2014; Solsvik and Jakobsen, 2015) and some others

investigated DSD regardless of the events happening to each droplet (Boxall et al., 2010; Calabrese et al., 1986; Coulaloglou and Tavlarides, 1977, 1976; Narsimhan et al., 1980; Ohtake et al., 1987; Wang and Calabrese, 1986). In addition, there are some additional studies, where computational fluid dynamic (CFD) in combination with PBE modelling is performed to predict the PSD of liquid-liquid emulsions (Agterof et al., 2003; Roudsari et al., 2012).

PBE is commonly used to take account for the break up and coalescence of the droplets, although it is computationally not affordable to consider the different slip velocities of the different droplet sizes. Furthermore, the PBE requires kernels for breakup and coalescence, which are difficult to obtain due to finding the parameters such as the breakage frequency (Ramkrishna, 2000).
In the current work, a hybrid approach is proposed, which combines the Eulerian-Eulerian two fluid model (TFM) and the Lagrangian discrete particle model (DPM) (Schneiderbauer et al., 2016a, 2016b). Here, the breakup of the droplets can be evaluated based on individual representative droplets. Moreover, hybrid TFM-DPM strategy has the advantage to acquire the Sauter mean diameter from DPM side (Lagrangian) and deliver it to TFM in order to calculate the accurate interphase momentum exchange term (Schneiderbauer et al., 2015). However, this hybrid approach requires the local equilibrium droplet size distribution. In the literature there are correlations, which evaluate the global Sauter mean diameter in a stirred tank reactors. The early stage correlation was developed based on the Kolmogorov length scale (Kolmogorov, 1941) by the work of Shinnar and Church (Shinnar and Church, 1960) and Chen and Middleman (Chen and Middleman, 1967) which reads,

$$\frac{D_{32}}{L} = AWe^{-0.6} \tag{1}$$

There are similar works available, which give different correlations for the global Sauter mean diameter (Calabrese et al., 1986; Coulaloglou and Tavlarides, 1976; Wang and Calabrese, 1986). However, there is no available local correlation for Sauter mean diameter based on the local fluid dynamic parameters (such as turbulence dissipation rate, ε) as it is difficult to obtain. Therefore, we investigated the droplet breakup in a Taylor-couette flow, in which the measurement of fluid dynamic parameters such as shear rate is well defined (Farzad et al., 2016). The resulting correlation depends on the shear rate and the fluid physical properties like density, viscosity and interfacial tension which is written as below (Farzad et al., 2016),

$$\frac{D_{32}}{h} = We^{-\frac{1}{6}}\,\mathrm{Re}^{-\frac{1}{4}}\left(\frac{\mu_d}{\mu_c}\right)^{0.33}\left(\frac{\rho_d}{\rho_c}\right)^{-6.6}$$
$$We = \frac{\rho_c a^2 h^3}{\gamma} \quad \mathrm{Re} = \frac{\rho_c a h^2}{\mu_c} \tag{2}$$

Note that, the power of h becomes zero due to combination of the h, Weber number and Reynolds number. Therefore, the normalized Sauter mean diameter is independent of the characteristic length (h).
Finally, while the modelling of breakup can be efficiently realized on a droplet level, the coalescence of the droplets would require resolving the collisions between individual droplets. In the following, we present novel models for breakup and coalescence. On the one hand, the breakup model is connected to equation (2) and on the other hand, the coalescence model represents a different discretization strategy of the population balance equations.

DROPLET BREAKUP MODEL

The present breakup model depends on the local Sauter mean diameter (equation 2), which can be obtained by using the local shear rate and the system's physical properties. Furthermore, our in-house experimental data (Farzad et al., 2016) reveals that the standard deviation scales linearly with the Sauter mean diameter, i.e. $\sigma = 0.33 D_{32}$, and that the DSD follows a log-normal distribution; this observation is also consistent with literature (Boxall et al., 2010). Therefore, the full local equilibrium DSD can be determined by using the Sauter mean diameter form the correlation (equation 2) and $\sigma = 0.33 D_{32}$. Thus, if a droplet is much larger than the the mean droplet size given from the DSD it might be prone to breakup. In this work, we employ the D_{90} for this threshold, which can be computed in each computational cell from the corresponding local DSD (Figure 1). If a droplet is larger D_{90} we sample a random number following the log-normal distribution. Only if this random number is larger than D_{90} as well, the droplet will break into two daughter droplets, where the diameter of the first daughter droplet is given by a second random number following the log-normal distribution. Note that, based on our assumption the local droplets (parcels) which are smaller than D_{90} remain stable as they are inside the local size distribution. Therefore, the local size distribution is constant and global size distribution changes till it reaches a steady state. Consequently, the diameter of the second daughter droplet can be easily computed from the volumes of the mother droplet and the first daughter droplet. This model was implemented as a user-defined function (UDF) to be used in the ANSYS FLUENT. The numerical implementation scheme will be discussed later. Note that breakup is not resolved for each droplet as it computationally costly and in most of the cases impossible; therefore, DPM uses parcels instead of particles which represent a group of particles with the identical diameter to reduce the computational costs.

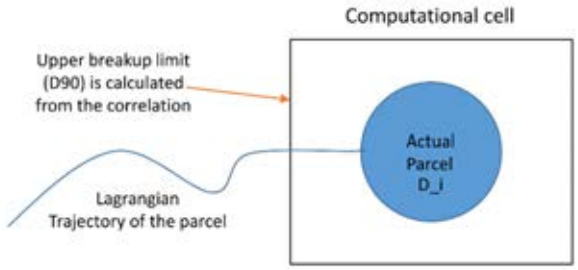

Figure 1: Schematic view of Lagrangian parcel which enters a specific computational cell with an upper breakup limit. If the parcel is larger than the limit then it breaks; otherwise, it remains unchanged.

DROPLET COALESCENCE MODEL

Modelling coalescence is more demanding compared to the breakup. Coalescence can be thought as the combination of collision frequency $\varsigma(d,d')$ and coalescence efficiency $\lambda(d,d')$. Thus, a general form of the coalescence frequency reads (Coulaloglou and Tavlarides, 1977; Leng and Calabrese, 2004),

$$\Gamma(d,d') = \varsigma(d,d')\lambda(d,d') \qquad (3)$$

Computing the collision frequency directly from droplet interactions is computationally very demanding and would decline the benefits of the hybrid approach. Therefore, we follow Coulaloglou and Tavlarides (Coulaloglou and Tavlarides, 1977), who defined the collision frequency and coalescence efficiency as below:

$$\varsigma(d,d') = c_1 \frac{\varepsilon^{1/3}}{1+\phi}(d+d')^2(d^{2/3}+d'^{2/3})^{1/2} \qquad (4)$$

$$\lambda(d,d') = \exp(-c_2 \frac{\mu_c \rho_c \varepsilon}{\sigma^2(1+\phi)^3}(\frac{d.d'}{d+d'})^4) \qquad (5)$$

Coalescence may occur when at least two droplets collide with each other; however, as noted above computing Γ from the interactions of the Lagrangian parcels would considerably decrease the computational efficiency of the present model. Thus, a different strategy is required to compute the rate of coalescence for the actual Lagrangian parcel. This strategy is outlined in the following: First, similar to PBE modelling we introduce a specific number of diameter classes. For each of this diameter classes, we are able to compute the corresponding volume fraction from mapping the data coming from the Lagrangian parcels to the Eulerian grid used for the TFM solution. Second, based on these "imaginary coalescence partners" given from this binning, we are able to compute the individual rates of coalescence (equation (3)). Note that the representative diameter of each bin is given by its mid diameter. Therefore, if we have N parcels and M bins in a cell, there are M×N combinations (e.g. $N \approx 2 \times 10^6$ $M = 13$). Third, the amount of volume created due to coalescence is locally stored regarding to its new diameter class in the appropriate diameter bins. Note that all the coalescence which can produce droplets larger than local D_{90} were neglected in order to reduce the computational cost as they are prone to breakup again in the next time step.

After storing the volume of the created droplets, they should be off loaded correctly into the available parcels with appropriate diameter. The volume remains stored until an appropriate parcel enters the computational cell; this procedure is known as "Bus stop model" (Schellander et al., 2012). Bus stop model helps to reduce the computational cost since always injecting the coalescence volume as a new parcel increases the computation time. However, there might be no suitable parcel available (regarding to its diameter class) in the surrounding; then, a new parcel should be injected in the next time step (flow time).

Two-fluid Model (TFM)

Resolving the motion of all droplets are computationally costly; therefore, it is more realistic to consider the averaged equation of motion and treat them as an Eulerian phase (Crowe et al., 2011). Continuity and momentum equations for the dispersed phase read (Ranade, 2001),

Continuity equation

$$\frac{\partial}{\partial t}(\alpha_d \rho_d) + \nabla.(\alpha_d \rho_d \vec{u}_d) = 0 \qquad (6)$$

Momentum equation

$$\frac{\partial}{\partial t}(\alpha_d \rho_d \vec{u}_d) + \nabla.(\alpha_d \rho_d \vec{u}_d \vec{u}_d) = -\alpha_d \nabla p + \nabla.(\alpha_d \tau_d) + F_d + \alpha_d \rho_d g \qquad (7)$$

F_d which denotes the interphase momentum exchange between the dispersed phase and the continues phase reads,

$$F_d = K_{cd}(\vec{u}_c - \vec{u}_d) \qquad (8)$$

In reality most of the dispersed multiphase flows such as droplets and particles are poly-disperse; therefore, Sauter mean diameter is required to calculate the interphase momentum exchange properly (Schneiderbauer et al., 2015).

Continuity and momentum equations for the continuous phase in a similar manner. This Eulerian-Eulerian approach is also known as TFM.

Discrete phase model (DPM)

This model provides the movement of a single or a cluster of particles (parcel) and tracks them in the flow field. Tracking the parcel trajectories gives the Lagrangian information. The momentum equation for the parcel trajectory is,

$$\frac{\partial}{\partial t}(u_{p,k}) = F_k^{poly} + g \qquad (7)$$

Hybrid model

Combining Lagrangian and Eulerian models yields the hybrid model. The TFM model predicts the flow field by

solving the Navier-Stokes equation and the DPM model passes the extra information (e.g. Sauter mean diameter) to the TFM part in order to improve the accuracy of the Eulerian part (Schneiderbauer et al., 2015). Furthermore, sensitivity analysis on several numerical settings reveals that the hybrid model is reliable (Schneiderbauer et al., 2016b).

This model is able to calculate the local Sauter mean diameter which changes the poly-disperse drag force (Figure 2). The modified Lagrangian trajectory can be written as below (Schneiderbauer et al., 2016a) ,

$$\frac{\partial}{\partial t}(u_{p,k}) = -\frac{1}{\tau_{col.d}}(u_{p,k} - \tilde{u}_d) + F_k^{poly} + g \qquad (7)$$

Figure 2: Single Lagrangian parcel trajectory (left side), the continuous droplets travels with local average velocity (middle), hybrid model in which consider the impact of the other existing droplets on the Lagrangian trajectory (right side)

RESULTS AND DISCUSSION

The numerical work by Roudsari et al. (Roudsari et al., 2012) and the experimental data by Boxall et al. (Boxall et al., 2010) were used to validate the proposed models. These works are similar; however, the first one (Roudsari et al., 2012) explains the CFD simulation of the water-in-oil emulsion in stirred tank by applying PBE and validating their results by the second paper (Boxall et al., 2010) which contains the experimental data. The so called Conroe oil was used as the continuous phase and distilled water as the dispersed phase (Boxall et al., 2010). The Conroe oil density, viscosity and interfacial tensions are 842 kg/m^3, 3.1 cP and 20 mN/m, respectively. The same geometry was used as Roudsari et al. (Roudsari et al., 2012). However, they used multiple reference frame (MRF) to simulate the impeller's rotation and ran the simulation in steady state but in the current work, dynamic simulation in combination with sliding mesh (SM) was carried out. Hexahedral mesh (Figure 3) of stirred tank reactor (Rushton turbine 6 blades and 4 baffles) was generated by using ANSYS ICEM (260,000 cells).

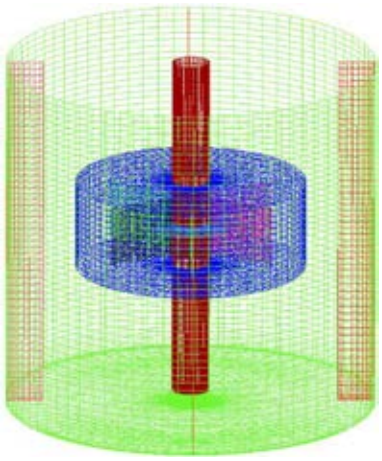

Figure 3: Stirred tank reactor mesh

As noted above, the Sauter mean diameter correlation, the breakup and the coalescence models were implemented as a UDF. The simulation of liquid-liquid system in stirred tank reactor including the hybrid TFM-DPM in combination with k-ε turbulence model was carried out by ANSYS FLUENT16.2. The time step size was 0.01s.

Breakup

The correlation of Sauter mean diameter (equation 2) was determined based on the dilute oil-water system (dispersed phase volume fraction was 1%) (Farzad et al., 2016); however, the volume fraction of dispersed phase in the experimental work of Boxall et al. (Boxall et al., 2010) is 15% and it can increase the Sauter mean diameter of the droplets due to coalescence (Coulaloglou and Tavlarides, 1976). Therefore, a linear correction factor was defined in the UDF based on the local volume fraction of the secondary phase in order to modify the correlation (equation 2) (Coulaloglou and Tavlarides, 1976) .

$$D_{32}^{'} = (1 + n\phi) D_{32}, \qquad (8)$$

where n is set to 6.5. Simulation was ran for two rotational speeds, 300 RPM and 600 RPM. The initial droplets with diameter of 0.6 mm and 0.3 mm were injected at t=0 for the 300 RPM (Figure 4) and the 600 RPM (Figure 5) cases, respectively.

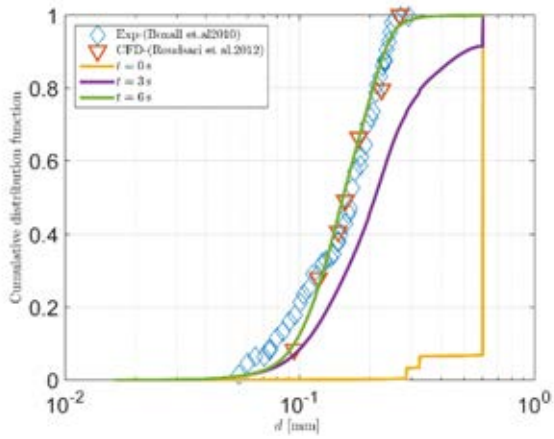

Figure 4: Cumulative drop size distribution at 300 RPM -Water in Conroe oil - Curves show the DSD (simulated) at t=0, 3 and 6 second- shaped scattered experimental data are taken from Boxall et al. (Boxall et al., 2010)- Nabla shaped points are CFD simulation results taken from Roudsari et al. (Roudsari et al., 2012)

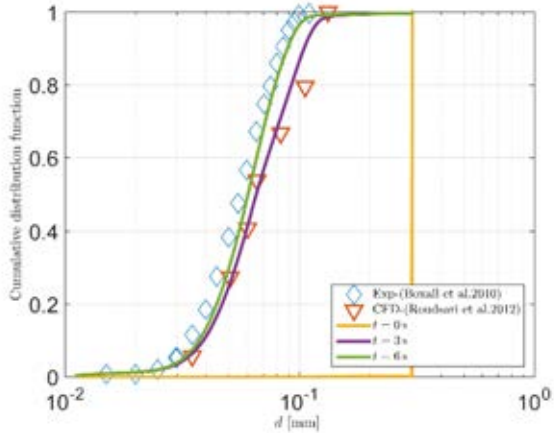

Figure 5: Cumulative drop size distribution at 600 RPM -Water in Conroe oil - Curves show the DSD (simulated) at t=0, 3 and 6 second-Diamond shaped scattered experimental data are taken from Boxall et al. (Boxall et al., 2010)- Nabla shaped points are CFD simulation results taken from Roudsari et al. (Roudsari et al., 2012)

As it can be seen from figure 4 and 5, the final status of the simulated results are in a good agreement with the experimental data (Boxall et al., 2010). Comparing the figures at t=3s (real flow time) reveals that the simulation at 600 RPM reached faster to its final state is compared to the 300 RPM. Therefore, mixing process is happening faster at 600 RPM in comparison with 300 RPM. However, studying the mixing time is not in the scope of this work. In addition, simulated DSD at 600 RPM follows the experimental data (Boxall et al., 2010) more accurately than compared to the simulated data provided by Roudsari et al. (Roudsari et al., 2012). Furthermore, using Lagrangian tracer trajectories provides the possibility to distribute the final simulated results into a large number of bins (400) in order to get smooth DSD. Roudsari et al. (Roudsari et al., 2012) used 7 bins as a part of PBE model available on the ANSYS FLUENT; therefore, their results are not as smooth as the results in the current work.

Coalescence

In order to validate the coalescence model, we study a process dominated by droplet coalescence. For example, when reducing the rotational speed was reduced from 600 RPM to 300 RPM breakup becomes negligible compared to coalescence. Nevertheless, both the breakup and the coalescence models were involved in this part of the simulation. The constant values of collision frequency, $c_1 = 1.29e^{-5}$ and coalescence efficiency, $c_2 = 7.32e^{12}$ were selected from (Maaß et al., 2007). However, the constant for the collision frequency was increased to $c_1 = 1$, in order to speed up the simulation to obtain the preliminary results. Figure 6 illustrates initial results of the coalescence model, where the curve at t=0 is the DSD at 600 RPM and after 0.5s (real flow time) DSD is almost close the experimental data at 300 RPM (Boxall et al., 2010).

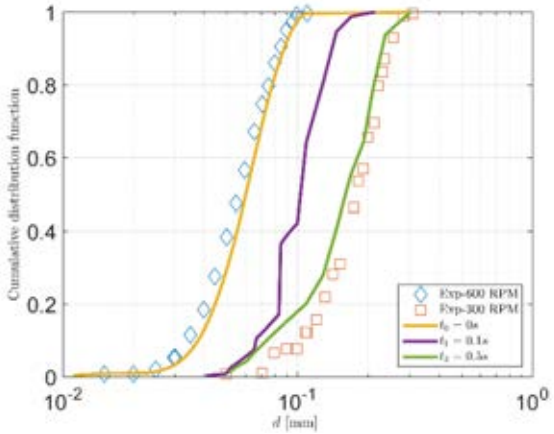

Figure 6: Cumulative drop size distribution evolves by time from 600 RPM to 300 RPM due to coalescence -Water in Crone oil - Curves show the DSD (simulated) at t=0, 0.1 and 0.5 second-Diamond shaped and square shaped scattered experimental data are taken from Boxall et al. (Boxall et al., 2010)

CONCLUSION

In this work, we presented novel breakup and coalescence models for liquid-liquid emulsions in combination with and Euerlian-Lagrangian Hybrid model. The main advantage compared to state of the art PBE modelling approaches is the Lagrangian nature of our approach, which allows the simple evaluation of, for example, residence time distribution.

The breakup model is based on an in-house correlation for Sauter mean diameter (Farzad et al., 2016), while the coalescence model is based on literature correlations. These models were combined with a hybrid TFM-DPM strategy, which allows the efficient analysis of poly-disperse systems. Final results for breakup show that the breakup model works fairly well for the validation case (Boxall et al., 2010; Roudsari et al., 2012). The initial results for the coalescence model are in a good agreement with the experiment (Boxall et al., 2010). However, these models, especially the model for coalescence require further investigation and more validation cases. Especially, larger systems will be subject to future investigations.

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