Proceedings of the 12th International Conference on
Computational Fluid Dynamics in the Oil & Gas,
Metallurgical and Process Industries

Progress in Applied CFD – CFD2017

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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 MODELING OF DYNAMIC EMULSION STABILITY

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ABSTRACT

Assuring transport and separation of oil and water crude emulsions is of significant importance to the oil and gas industries. The crude oil, due to its profuse chemical composition, has complex dispersion and emulsion flow behavior with water. As a result, of the interface chemistry, the bubbles and droplets may separate easily, or not separate at all, impacting flow regime, water holdup, pressure drop and separation efficiency during pipe transport. Using a recently developed new stirred tank characterization technique for emulsion stability droplet relaxation parameters can be studied. Multiple model oils and crude oils were characterized by this technique. This work discusses development of a pragmatic modeling method that can validate the experimental measurements. A time averaged velocity profile in a stirred tank is used to obtain a 1-D flux flow profile in the vertical direction. This 1-D flux profile is used as a simplified flow equation and scalar equations for droplet size and dispersed phase fraction is used for modeling the emulsion stability and relaxation. This method can help in fast simulation of emulsion stability that involves long time scales of coalesence and breakage evolution for crude oil and water.

Keywords: Multiphase flow, oil-water emulsion, flow assurance.

NOMENCLATURE

A complete list of symbols used, with dimensions, is required.

Greek Symbols
ρ Mass density, [kg/m^3].
μ Dynamic viscosity, [kg/m.s].
Γ Dispersed phase viscosity, [m^2/s].
Ω relaxation coefficient, [1/s].

Latin Symbols
a Characteristic area, [m^2].
p Pressure, [Pa].
$\mathbf{u}$ Velocity, [m/s].

$\overline{U}$ Averaged velocity, [m/s].
$\overline{d}$ mean droplet size, [m].
$\overline{\alpha}$ dispersed phase fraction, [-].
$\overline{V}$ Dispersed phase velocity, [m/s].
τ Relaxation time scale for droplets, [s].

Sub/superscripts
c   Continuous phase.
A   upward flow direction.
B   downward flow direction.
E   Exchange flow between A and B.
z   z- direction representing height direction of tank
eq Equilibrium

INTRODUCTION

The pipeline transport of crude oil-water dispersions or emulsions is typical for many oil fields and flow assurance studies has been hampered by limited understanding of how to handle the possible behavior of the flow when stabilizing surfactants are present. The cost of crude oil production is strongly related to pressure drop produced in transport pipes. It is well known that pressure drop is strongly dependent on the rheological behavior, which is strongly influenced by emulsion stability. Therefore oil-water emulsion stability has been a subject to several studies in the past.

Emulsion stability or droplet size evolution is strongly influenced by interfacial tension (IFT) and surface chemistry (Aichele 2009; Mullins et. al. 2007; Sjoblom 2005). So there has been a need to quantify the droplet size evolution behaviour for given characteristics of oil-water emulsions. This has been achieved by an advanced imaging technique developed recently and presented in Patil at. al. (2017). In this method, the measurement of droplet size alongside torque provides the necessary understanding of dissipation on emulsion stability.

Experiments with model oils-water emulsion has shown that the droplet size in turbulent regimes is governed by Kolmogorov scale criteria (Kolmogorov, 1949). Depending on the regime defined by the inertial and viscous subrange; the equilibrium droplet size agree well with the theoretical correlations (Boxall et. al.

2010; Boxall et. al. 2012; Patil et. al. 2017). Further the dynamic droplet size relaxation of emulsions have also been studied by measuring the time dependent droplet relaxation and hence its coefficient (Calderbank, 1958; Patil et. al., 2017).

Dispersion of two phases by emulsification in a stirred tank has long been modeled using various multiphase modelling methods. Most common models for such fluid-fluid systems is the Euler-Euler method (Murthy et. al. 2007). Besides CFD methods using Population Balance models (PBM) to represent the dynamic dispersed phase have also been developed (Trætli-Einarsrud et. al. 2014, Raikar et. al. 2009).

Generally for model oil-water emulsions the time scales for relaxations is several seconds (Patil et. al. 2017). For crude oil-water emulsions which have stabilizing components these time scales are higher (few minutes) (Patil et. al. 2017b). The challenges with using Euler-Euler methods (in 3D) is that they are slow and time consuming due to the small time steps needed ($<10^{-4}$s). The CFD-PBM approach is still a useful modelling method. But a number of challenges were encountered in using such a method for emulsions where surface active components influence the droplet behavior.

For a normal stirred tank cell with a single impeller the radial and angular variation in dissipation is very small relative to the height. Therefore, a pragmatic 1-D model in height direction can make the model simplistic and fast. This will essentially also make emulsion stabilization modelling easy. Initially only the Sauter mean diameter (SMD) of the droplet will be modelled and later a size distribution model can be developed with a PBM kind of technique, like in Einarsrud et. al. (2014). In this work we describe the development of such a pragmatic 1-D model.

MODEL DESCRIPTION

The oil and water phase in the emulsion stability study are of nearly the same density and hence the 3-D flow patterns in the tank will not be much different from a single phase flow. So the flow pattern for the 3 speed levels of impeller can be evaluated using a single phase flow simulations. The properties of the continuous phase can be used for such a simulation.

The continuity and momentum equation for the 3D system is represented by;

$$\frac{\partial \rho_c}{\partial t} + \nabla \cdot \left(\rho_c \widetilde{\mathbf{u}}_c \right) = 0 \tag{1}$$

$$\frac{\partial \rho_c \widetilde{\mathbf{u}}_c}{\partial t} + \nabla \cdot \left\{ \left(\rho_c \widetilde{\mathbf{u}}_c \widetilde{\mathbf{u}}_c \right) + \left(\overline{\rho_c \mathbf{u}''_c \mathbf{u}''_c} \right) - \tau_c \right\} = -\nabla p + \rho_c g \tag{2}$$

Where, ρ_c is the density of continuous phase. Turbulent fluctuations are modelled with the k-ε model.
In these single phase simulations the impeller blade moments is integrated to obtain the torque. The torque is

monitored till equilibration is achieved. The simulation is continued further by time averaging the velocity field to obtain the averaged flux.

It is well known that the averaged velocity field for a baffled and flat blade impeller based stirred tank has a profile that looks like in Fig. 1. There are 2 circulation currents in the vertical z-direction. Both currents start at the impeller in radially outward direction. This results in a two large scale counter-rotating vortices. The upper vortex is moving up along the wall, above the impeller, while the lower vortex moving down along the wall, below the impeller. The flow recirculates back along the shaft as shown in Fig. 1. The upwards and downwards flow field sections is shown in Fig. 1 where the areas are marked. Within this flow pattern note that the upward and downward flow mass rate is always the same. The difference in the area is balanced by difference in mean velocities (z-directional).
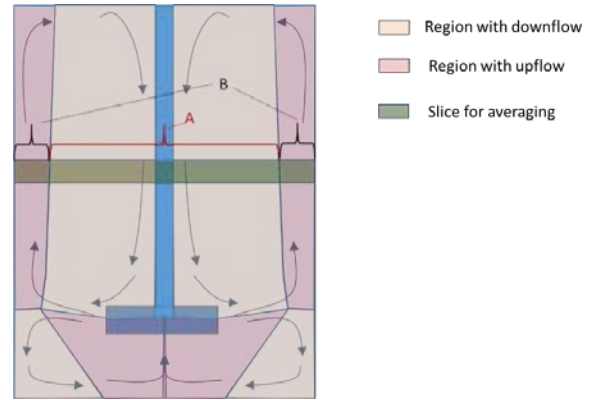
Figure 1: Regions with upward and downward flows are marked

This 3-D time averaged velocity field data is utilized to obtain a pseudo 1-D flow field in the vertical direction (z-direction) and horizontal directions. For this purpose, the flow fields in the cross section is averaged for upward and downward flow defined by region A and B at discrete cross sections along the z direction. Thus the upward and downward mean velocity and the upward and downward, and the corresponding cross sectional areas are evaluated. The averaged upward and downward velocity is given by;

$$\overline{U_A} = \frac{\int_A u_{c,z} da}{\int_A da} \text{ and } \overline{U_B} = \frac{\int_B u_{c,z} da}{\int_B da} \tag{3}$$

Where, $u_{c,z}$ is the z-direction component velocity of the fluid velocity field $\widetilde{\mathbf{u}}_c$. The flow area for the streams A and B are given by;

$$a_A = \int_A da \text{ and } a_B = \int_B da \tag{4}$$

For evaluation of the average turbulent dissipation ε in horizontal slices, denoted A and B we define:

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$$\overline{\varepsilon}_A = \frac{\int_A \varepsilon dV}{\int_A dV} \quad \text{and} \quad \overline{\varepsilon}_B = \frac{\int_B \varepsilon dV}{\int_B dV} \tag{5}$$

These dissipations rates, averaged over horizontal slices with finite thickness Δz, are critical input for evaluation of the equilibrium droplet sizes used by the model.
The mass conservation on a slice, for the zones A and B, is then given by:

$$\left[a_A \overline{U_A}\right]_{z^-}^{z^+} - U_E a_I = 0$$
$$\left[a_B \overline{U_B}\right]_{z^-}^{z^+} + U_E a_I = 0 \tag{6}$$

Here U_E is the average radially directed velocity (horizontal exchange velocity), communicating through area A_I, which is easily determined based on the interface location between zones A and B. The radial velocity U_E can be computed from any of the two relations in Eq.(6).
The above description for total flow balance is summarized in Fig. 2. It is to be noted that for each tank cross sectional area, the upward and downward volumetric flow is the same. This means that;

$$\overline{U_{A,k+\frac{1}{2}}} \, \overline{a_{A,k+\frac{1}{2}}} = \overline{U_{B,k+\frac{1}{2}}} \, \overline{a_{B,k+\frac{1}{2}}} \tag{7}$$

This is consistent with the global mass conservation equations, Eq. (6)
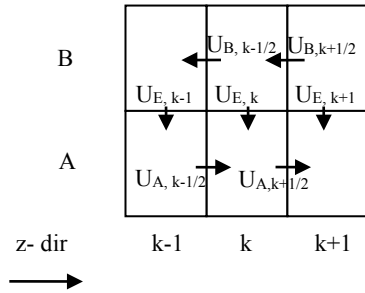
Figure 2: Grid description for the 1-D model

This 1-D averaged data is utilized in the dynamic droplet size model equation provided by;

$$\frac{\partial}{\partial t} a_A \overline{d_{A,z}} + \frac{\partial}{\partial z}\left(a_A V_z \overline{d_{A,z}}\right) = \frac{\partial}{\partial z} \Gamma a_A \frac{\partial \overline{d_{A,z}}}{\partial z}$$
$$+ a_A \frac{\overline{d_{eq,A,z}} - \overline{d_{A,z}}}{\tau} + \Omega a_I \left(\overline{d_{B,z}} - \overline{d_{A,z}}\right) \tag{8}$$
$$+ \frac{a_I}{\Delta z}\left(\max(U_E,0)\overline{d_{B,z}} - \max(-U_E,0)\overline{d_{A,z}}\right)$$

The above equation formulation is a passive scalar transport equation with source terms. The 3-D version of this can be found in Laux and Johansen (1999). Similarly for the droplet size in zone B:

$$\frac{\partial}{\partial t} a_B \overline{d_{B,z}} + \frac{\partial}{\partial z}\left(a_B V_z \overline{d_{B,z}}\right) = \frac{\partial}{\partial z} \Gamma a_B \frac{\partial \overline{d_{B,z}}}{\partial z}$$
$$+ a_A \frac{\overline{d_{eq,B,z}} - \overline{d_{B,z}}}{\tau} - \Omega a_I \left(\overline{d_{B,z}} - \overline{d_{A,z}}\right) \tag{9}$$
$$- \frac{a_I}{\Delta z}\left(\max(U_E,0)\overline{d_{B,z}} - \max(-U_E,0)\overline{d_{A,z}}\right)$$

Where; $\overline{d_{A,z}}$ is the averaged droplet size in the zone of upward flow at position z. The above 1-D model is further simplified by neglecting the shear term defined by the viscosity of the continuous phase. Since this model is not taking the detailed flow into consideration the shear effect can be essentially lumped into Equilibrium droplet size $\overline{d_{eq,A,z}}$. The $\overline{d_{eq,A,z}}$ is a function of multiple factors defined by fluid properties and the presence of surface-active components. If the surface-active components are not present then depending on the flow regime the droplet size is governed by inertial or viscous sub-range correlations in (Patil et. al. 2017).
In these two equations ((8),(9)) Ω is a dispersion transfer coefficient, expressing the turbulence induced exchange rate of particle size between the two zones. The last term in Eqs. (8) and (9) express the convective transport between zones A and B.

The droplet fraction in zone A is conserved by:

$$\frac{\partial}{\partial t} a_A \overline{\alpha_{A,z}} + \frac{\partial}{\partial z}\left(a_A V_z \overline{\alpha_{A,z}}\right) = \frac{\partial}{\partial z} \Gamma a_A \frac{\partial \overline{\alpha_{A,z}}}{\partial z}$$
$$+ \Omega a_I \left(\overline{\alpha_{B,z}} - \overline{\alpha_{A,z}}\right) \tag{10}$$
$$+ \frac{a_I}{\Delta z}\left(\max(U_E,0)\overline{\alpha_{B,z}} - \max(U_E,0)\overline{\alpha_{A,z}}\right)$$

The above equation is a general mass conservation equation for dispersed phase assuming phase densities are constant. It is averaged over all the control volumes in the system. Similarly for zone B, we have

$$\frac{\partial}{\partial t} a_B \overline{\alpha_{B,z}} + \frac{\partial}{\partial z}\left(a_B V_z \overline{\alpha_{B,z}}\right) = \frac{\partial}{\partial z} \Gamma a_B \frac{\partial \overline{\alpha_{B,z}}}{\partial z}$$
$$+ \Omega a_I \left(\overline{\alpha_{B,z}} - \overline{\alpha_{A,z}}\right) \tag{11}$$
$$- \frac{a_I}{\Delta z}\left(\max(U_E,0)\overline{\alpha_{B,z}} - \max(U_E,0)\overline{\alpha_{A,z}}\right)$$

The dispersed phase velocity in z-direction V_z has essentially two components, which are convective velocity U_z and terminal velocity.

$$V_z = U_z + V_t \tag{12}$$

Here V_t is the dispersed phase velocity component from Stokes law given by;

$$V_t = \frac{(\rho_c - \rho_d)d^2 g}{18\mu} \tag{13}$$

Further discretization and rearranging Eq. (8) gives the following equation to solve the (Sauter mean) droplet size equations in height direction.

$$\frac{a_A}{\Delta t}(\overline{d_{A,n+1}} - \overline{d_{A,n}}) + \frac{1}{\Delta z}\left[a_A\left(\overline{U_A} + \overline{V_t}\right)\overline{d_{A,z}}\right]_{z^-}^{z^+} =$$

$$\frac{1}{\Delta z}\left[\Gamma a_A \frac{\partial \overline{d_{A,z}}}{\partial z}\right]_{z^-}^{z^+} \qquad (14)$$

$$+ a_A \frac{\overline{d_{eq,A,z}} - \overline{d_{A,z}}}{\tau} + \Omega a_I\left(\overline{d_{B,z}} - \overline{d_{A,z}}\right)$$

$$+ \frac{a_I}{\Delta z}\left(\max(U_E, 0)\overline{d_{B,z}} - \max(-U_E, 0)\overline{d_{A,z}}\right)$$

In equations (15) and (16) the notation z^+ and z^- denotes the cell boundary positions for the slice where the droplet size is computer. The averaged velocities U_A and U_B are always computed at these cell boundaries (staggered grid arrangement).

Before proceeding, we subtract the product of droplet size and fluid mass conservation eq. (6), and rearrange.

$$\frac{a_{A,k}}{\Delta t}(\overline{d_{A,k,n+1}} - \overline{d_{A,k,n}}) + \frac{1}{\Delta z}\left(a_{A,k}\overline{U_{A,k}}\right)^+\left(\overline{d_{A,k,n}}^{z^+} - \overline{d_{A,k,n}}\right)$$

$$- \frac{1}{\Delta z}\left(a_{A,k}\overline{U_{A,k}}\right)^-\left(\overline{d_{A,k,n}}^{z^-} - \overline{d_{A,k,n}}\right)$$

$$+ \frac{1}{\Delta z}\left[\left(a_A\overline{V_t}\right)^+ \overline{d_{A,k,n}}^{z^+} - \left(a_A\overline{V_t}\right)^- \overline{d_{A,k,n}}^{z^-}\right] = \qquad (15)$$

$$\frac{1}{\Delta z}\left[\Gamma_k a_{A,k} \frac{\partial \overline{d_{A,k,n}}}{\partial z}\right]_{z^-}^{z^+} + a_{A,k}\frac{\overline{d_{eq,A,k,n}} - \overline{d_{A,k,n}}}{\tau}$$

$$+ \Omega_k a_{I,k}\left(\overline{d_{B,k,n}} - \overline{d_{A,k,n}}\right)$$

$$+ \frac{a_{I,k}}{\Delta z}\left(\max(U_{E,k}, 0)\left(\overline{d_{B,k,n}} - \overline{d_{A,k,n}}\right)\right)$$

The values at the cell faces ($\overline{d_{A,z}}^{z^+}$ and $\overline{d_{A,z}}^{z^+}$) are now approximated by the upwind value, controlled by U_A or the terminal velocity V_t.

Note that here by convention, $\overline{U_{A,k}}$ and $\overline{U_{B,k}}$ are always positive representing the upward and downward velocity direction respectively. However, $\overline{V_t}$ and $\overline{U_E}$ can be positive or negative depending on density difference and direction of the flow respectively. If continuous phase density is larger than dispersed phase $\overline{V_t}$ is positive (in z direction). Else it is negative when dispersed has higher density.

At any given cross sectional grid say 'k' in z direction, if the exchange of mass is from B zone (downward flow) to A zone (upward flow) then the $\overline{U_{E,k}}$ is positive. Similarly, vis-versa it is negative.

$$\frac{a_{A,k}}{\Delta t}(\overline{d_{A,k,,n+1}} - \overline{d_{A,k,n}}) - \frac{1}{\Delta z}\left(a_{A,k}\overline{U_{A,k}}\right)^-\left(\overline{d_{A,k-1,n}} - \overline{d_{A,k,n}}\right)$$

$$+ \frac{1}{\Delta z}\left[\left(a_A\overline{V_t}\right)^+ \overline{d_{A,k,n}}^{z^+} - \left(a_A\overline{V_t}\right)^- \overline{d_{A,k,n}}^{z^-}\right] = \qquad (16)$$

$$\frac{1}{\Delta z}\left[\Gamma_k a_{A,k} \frac{\partial \overline{d_{A,k,n}}}{\partial z}\right]_{z^-}^{z^+} + a_{A,k}\frac{\overline{d_{eq,A,k,n}} - \overline{d_{A,k,n}}}{\tau}$$

$$+ \Omega_k a_{I,k}\left(\overline{d_{B,k,n}} - \overline{d_{A,k,n}}\right)$$

$$+ \frac{a_{I,k}}{\Delta z}\left(\max(U_{E,k}, 0)\left(\overline{d_{B,k,n}} - \overline{d_{A,k,n}}\right)\right)$$

Similarly, a formulation for the downward flow droplet size equation exists given by;

$$\frac{a_{B,k}}{\Delta t}(\overline{d_{B,k,n+1}} - \overline{d_{B,k,n}}) + \frac{1}{\Delta z}\left(a_{B,k}\overline{U_{B,k}}\right)^+ \left(\overline{d_{B,k+1,n}} - \overline{d_{B,k,n}}\right)$$

$$+ \frac{1}{\Delta z}\left[\left(a_B\overline{V_t}\right)^+ \overline{d_{A,k,n}}^{z^+} - \left(a_A\overline{V_t}\right)^- \overline{d_{A,k,n}}^{z^-}\right] = \qquad (17)$$

$$\frac{1}{\Delta z}\left[\Gamma_k a_{B,k} \frac{\partial \overline{d_{B,k,n}}}{\partial z}\right]_{z^-}^{z^+} + a_{B,k}\frac{\overline{d_{eq,A,k,n}} - \overline{d_{A,k,n}}}{\tau}$$

$$- \Omega_k a_{I,k}\left(\overline{d_{B,k,n}} - \overline{d_{A,k,n}}\right)$$

$$- \frac{a_{I,k}}{\Delta z}\left(\max(U_{E,k}, 0)\left(\overline{d_{B,k,n}} - \overline{d_{A,k,n}}\right)\right)$$

The conservation equations for the dispersed phase is given by eqs. (10) and (11). These equations as well, may be discretised, using explicit time integration and first order unwinding for convection.

It should be noted that the vertical dispersion coefficient Γ as well as the horizontal exchange coefficient Ω has not been determined yet. These may be estimated based on the mixing length hypothesis, or may be extracted from the CFD simulations. As a first approach we may neglect the effects of turbulent dispersion and convective dispersion will dominate in most cases.

Both the terminal velocity and the equilibrium size may be made explicitly depending on the droplet fractions. Accordingly, the terminal velocity V_t in equations (16) and (17), will depend on the solution of the droplet fraction equations (10) and (11).

For the top and bottom slices the boundary condition is that there is no flux of droplet size or droplet mass (volume fraction) across these external boundaries. The droplet fraction may build to large values in the end-of-domain cells. In this case over compaction may, as an example, be avoided by enforcing the droplet velocities to become stagnant at a maximum packing.

The 3-D single phase flow simulations of stirred tank was performed using ANSYS Fluent 17.1. The 3-D time averaged velocity field data was imported in MATLAB to obtain time averaged 1-D volumetric flow rate in height direction.

RESULTS

The averaged velocity vector plot for the 3-D flow field is shown hereby in Fig. 3 for a 3500 RPM impeller speed. This plot illustrates the flow field description provided earlier in the previous section Fig. 1.

The z-direction velocity field is shown in Fig. 4. Note that close to the impeller tip the fluid velocities are very high. Therefore, the scale in this fig has been limited to +1.5 and -1.5 m/s velocity range so that remaining flow features are better visible.
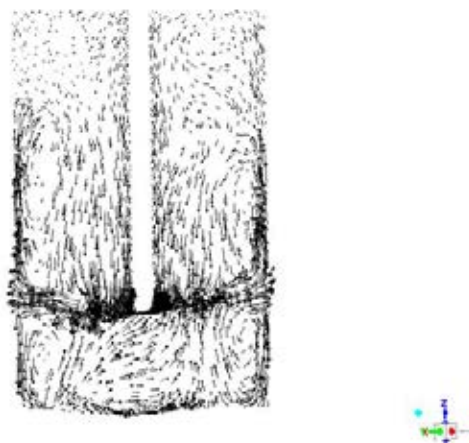
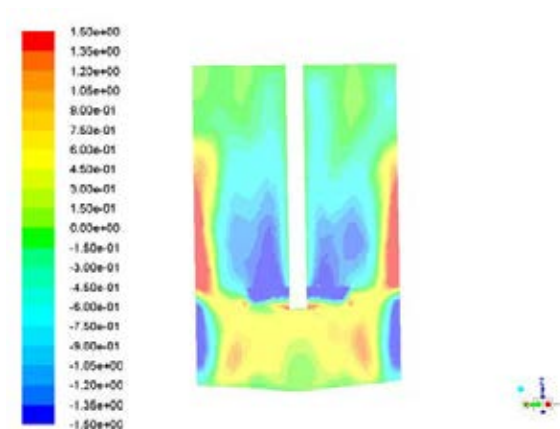**Figure 3:** Cross sectional cut view of velocity vector field

Figure 4: Cross sectional cut view of z-directional velocity colour profile

The data from the time averaging done over a 3-D simulation data for 25 s gave a profile that equilibrated and changed negligibly with time. Using this profile data the positive and negative averaged velocity fields were averaged at discrete cell faces in z direction. These cell face velocities are weighted with respect to cell face area as per Eq. (3) to give averaged upward and downward velocities.

Besides, integrating the upward and downward flow area provides averaged area of A and B. The volumetric flow rate in upward and downward direction can thus be obtained which both should be equal from Eq. (7).

Further using Eq. (6) the exchange velocity and volumetric flow rate between the two zones (A and B) can be obtained. The dimensions of the tank is summarized in Table 1.

Table 1: Model dimension.

Dimensions	
Tank diameter	0.095 m
Tank height	0.148 m
Impeller diameter	0.05 m
Number of cells in z direction	10
Grid size (z-direction)	0.0148 m

It is to be noted that though the averaging takes place for a long enough time there is always some small difference between the upward and downward flow rates. Though this numerical difference is negligibly small they need to be removed for the 1-D simulation as this may cause numerical leakages for the dispersed phase equation.

Therefore, the upward and downward volumetric flow rate are averaged out as a reasonable approximation. Fig. 5 shows a plot of the averaged upward and downward volumetric flow rate for the 3-D simulation at 3500 RPM impeller speed. These are at cell face positions. Besides, it also shows a plot of cell exchange flow rate between A and B zone at cell centre position.
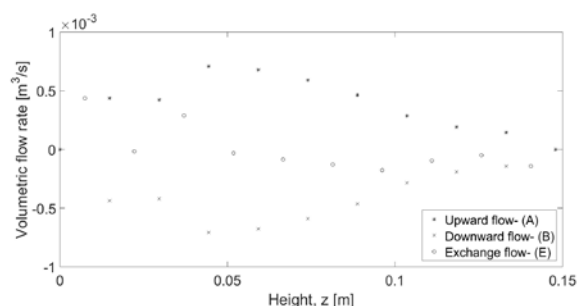

Figure 5: Upward and downward volumetric flow rate and exchange flow rate

This has provided a complete internally balanced velocity field that can be used for dispersed phase simulations. Using such a 1-D method, fast simulation of dispersed phase evolution is possible. With this method, the long time scales of emulsion droplet size relaxation can be modelled.

CONCLUSION

A simplified 1-D modelling method has been proposed to mimic emulsion stability in stirred tank. This method uses time averaged velocity fields from 3-D single phase simulations to obtain 1-D flow rate in z direction (upward and downward direction). This balanced flow rate field can be further used for modelling the size evolution of a dispersed phase in the height or z direction. Using such a method long time scales of emulsion evolution can be modelled fast. These models can be fitted with emulsion evolution parameters obtained experimentally using a stirred tank. Such models can in future be used in 1-D pipe simulation software.

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