Modelling of droplet breakup and coalescence in an oil-water pipeline

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Abstract

In dispersed two-phase flows, the particle size is probably the most important parameter in determining the particle dynamics. Interphase forces, heat and mass transfers are all functions of the particle diameter. Diameters of the particles are unlikely to be uniform and for droplets and bubbles they can change continuously due to breakup and coalescence. Methods of moments have been used very successfully in modeling particle size distributions in dispersed two-phase flows. The $S_f$ model described in this paper is based on the method of moment. It contains models for droplet breakup and coalescence.

For breakup, the model considers the balance between disruptive forces (due to shear and turbulence) and restoring forces (due to surface tension) on the droplet. In laminar flows the viscous effects dominate hence we named this regime “viscous breakup”. In turbulence flows the interactions with turbulence eddies dominate and we named this regime “inertia breakup”. For coalescence, the model considers the probability of collisions of the droplets, the contact time of two colliding drops and the drainage time of the liquid film between the drops. Similar to the breakup model, we have the “viscous collision” regime in laminar flows and the “inertia collision” regime in turbulent flows. The drainage time is a function of the state of the droplet surface, whether it is fully or partially mobile or totally immobile. The model therefore considers the breakup and coalescence processes in great details.

The $S_f$ model was implemented in the Eulerian multiphase flow model in the commercial CFD software, STAR-CD. The model was applied to analyse the oil-water pipeline experiment of Simmons and Azzopardi (2001). It was found that droplet breakup was strongest near the pipe walls since turbulence and velocity gradient were strongest there. Since horizontal pipe flow was considered, some settling of the water droplets (the heavier phase) was observed as in the experiments. The predicted droplet size distribution was found to be relatively insensitive to the initial droplet diameter specified at the pipe inlet. The computed and the measured droplet size distributions at the pipe exit were presented and compared in form of cumulative frequency curves. Reasonable agreements between the two sets of curves were obtained.

Introduction

In dispersed two-phase flows, the size distribution of the dispersed phase can undergo continuous change due to breakup, coalescence, agglomeration, growth, expansion, shrinkage, etc. Correct description of the size distribution is important in correctly simulating the two-phase flow behaviour. This paper describes the details of the $S_f$ model in the STAR-CD software, which was developed to model the size distribution of dispersed droplets and bubbles with the consideration of breakup and coalescence effects. This model was developed under a European Project, Brite/Euram BE 4322 (Vaessen 1998).

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$A_{II}$</td>
<td>Hamaker constant</td>
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<tr>
<td>$B$</td>
<td>Birth rate of particles (s$^{-1}$)</td>
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<td>$D$</td>
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<tr>
<td>$d$</td>
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<td>$h_{cr}$</td>
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<td>$K$</td>
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<td>$k_{br}$</td>
<td>Inertia breakup time constant</td>
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<td>$L_k$</td>
<td>Kolmogorov length scale (m)</td>
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<td>$M$</td>
<td>Moment of particle distribution</td>
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<td>$N$</td>
<td>Number of droplet</td>
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<td>$n$</td>
<td>Number density of particles</td>
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<td>$P_{coal}$</td>
<td>Coalescence probability</td>
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<td>$P(d)$</td>
<td>Particle distribution function</td>
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Droplet size distribution model

The evolution of the droplet size distribution as a result of coalescence and breakup can be modelled by means of the population balance equation (PBE). A simplified form of the equation for the size-i droplets can be written as:

$$\frac{Dn_i}{Dt} = B_{i,br} - D_{i,br} + B_{i,cl} - D_{i,cl} \quad (1)$$

where $n_i$ is the number density of the droplets in size-i group, $B_{i,br}$ and $D_{i,br}$ stand for birth and death of droplets due to breakup. Similarly $B_{i,cl}$ and $D_{i,cl}$ stand for birth and death of droplets due to coalescence.

A detailed description of the droplet size distribution will require a large number of population classes say 10 to 20. The computational effort required to solve 10 to 20 PBE’s simultaneously in a CFD calculation can be large.

A simpler alternative can be derived by assuming that the droplet size distribution conforms to a pre-defined shape, and this shape is retained during the process under investigation. Under these conditions, the complete droplet size distribution can be represented by a limited number of parameters and the PBE could be reformulated in terms of these parameters. $S_\gamma$ is conserved on a volumetric basis and is related to the moment $M_\gamma$ of the distribution:

$$S_\gamma = nM_\gamma = n \int_0^\infty d^3 P(d) d(d) \quad (2)$$

where $n$ is the total number density of the droplets, $n = S_0$. $S_\gamma$ is the local intensity of dispersion. If the distribution is characterised by $N$ parameters then $N$ independent intensities $S_\gamma$ are sufficient to describe the complete distribution.

The Sauter Mean diameter is therefore:

$$d_{32} = \frac{S_3}{S_2} \quad (4)$$

The $S_3$ is related to the volume fraction of the droplets $\alpha$:

$$\alpha = \left( \frac{\int_0^\infty d^3 P(d) d(d)}{\frac{\pi}{6}} \right) \quad (5)$$

The Sauter Mean diameter becomes:

$$d_{32} = \frac{6\alpha}{\pi} \frac{1}{S_2} \quad (6)$$

The transport equation for $S_\gamma$ is:

$$\frac{DS_\gamma}{Dt} = \frac{\partial S_\gamma}{\partial t} + \nabla S_\gamma u_d = s_{br} + s_{cl} \quad (7)$$

where $s_{br}$ and $s_{cl}$ are the source terms for breakup and coalescence respectively.

In many practical situations, the log-normal distribution can be used to characterise the droplet size distribution. The log-normal distribution is characterised by two parameters, a mean, $\bar{d}$, and a width, $\hat{\sigma}$:

$$P(d) = \frac{1}{d\hat{\sigma}\sqrt{2\pi}} \exp\left( -\frac{(\ln d - \ln \bar{d})^2}{2\hat{\sigma}^2} \right) \quad (8)$$

Since the log-normal distribution is characterised by two parameters, two independent $S_\gamma$ are required to described the distribution. $S_3$ is readily available from the volume...
fraction, shown in (5), only one transport equation for $S_γ$ needs to be solved. In order to obtain the Sauter Mean diameter, the $S_2$ equation is solved.

### Breakup model

The breakup source term in its generic form is given by:

$$s_{br} = \int_{0}^{\infty} K_{br}(d) \Delta S_{br}^{S_γ}(d) nP(d) d(d)$$  \hspace{1cm} (9)

where $K_{br}$ is the breakup rate, $\Delta S_{br}^{S_γ}(d)$ is the change in $S_γ$ due to a single breakup event of a droplet of size $d$.

An expression for $\Delta S_{br}^{S_γ}(d)$ follows from the conservation of dispersed phase volume during a breakup event:

$$N_f \frac{\pi d_f^3}{6} = \frac{\pi d^3}{6} \Rightarrow d_f = d \cdot N_f^{1/3}$$  \hspace{1cm} (10)

That is the breakup of a droplet of diameter $d$ resulting in $N_f$ droplets of diameter $d_f$.

The birth and death changes of $\Delta S_{br}^{S_γ}(d)$ due to breakup are:

$$\Delta S_{br}^{S_γ}(d) = N_f(d) d_f^3 - d^3 = d^3 \left( N_f(d) \frac{3}{3} - 1 \right)$$  \hspace{1cm} (11)

The breakup rate $K_{br}$ is equal to the reciprocal breakup time, $\tau_{br}$ . The breakup source term becomes:

$$s_{br} = \int_{0}^{\infty} \left[ \frac{d^3 \left( N_f(d) \frac{3}{3} - 1 \right)}{\tau_{br}(d)} \right] nP(d) d(d)$$  \hspace{1cm} (12)

Modelling is required for the parameters $N_f(d)$ and $\tau_{br}(d)$, as a function of the local flow conditions.

In the current implementation of the model, only binary breakup is considered in which droplets are broken into two fragments of equal size.

$$N_f(d) = 2$$  \hspace{1cm} (13)

### Breakup regimes

Breakup will occur only if the droplet is larger than the critical diameter, the so-called maximum stable droplet diameter. Viscous breakup is found in laminar flows, and in turbulent flows for droplets smaller than the Kolmogorov length scale. Larger droplets are subjected to inertial breakup.

The Kolmogorov length scale $L_k$ is given by:

$$L_k = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4}$$  \hspace{1cm} (14)

where $\nu$ is the kinematic viscosity and $\varepsilon$ is the dissipation rate of turbulent kinetic energy.

In the case of turbulent flow with $d_{cr} < L_k$ the breakup source term is given by the sum of the sources for the viscous ($d_{cr} < d < L_k$) and inertia ($d > L_k$) regimes:

$$s_{br} = s_{br,v} + s_{br,i}$$  \hspace{1cm} (15)

### Viscous breakup

The breakup criterion follows from a balance between disruptive and restoring forces: the viscous stress and Laplace pressure respectively. This force balance is expressed in terms of the capillary number, $\Omega$:

$$\Omega = \frac{\mu_c d\dot{\gamma}}{2\sigma}$$  \hspace{1cm} (16)

where $\mu_c$ is the dynamics viscosity of the continuous phase, $\dot{\gamma}$ is the shear rate, $\sigma$ is the surface tension coefficient.

Breakup condition is a function of the viscosity ratio between the phases and whether the flow is rotational or elongational. The breakup criterion is given as $\Omega \geq \Omega_{cr}$.

The critical diameter is therefore given by:

$$d_{cr} = \frac{2\sigma \Omega_{cr}}{\mu_c \dot{\gamma}}$$  \hspace{1cm} (17)

The shear rate, $\dot{\gamma}$, is calculated from the local velocity gradient for laminar flows and for turbulent flows the Kolmogorov shear rate is used:

$$\dot{\gamma}_k \equiv \sqrt{\frac{\varepsilon \rho_c}{\mu_c}}$$  \hspace{1cm} (18)

where $\rho_c$ is the density of the continuous phase.

From dimensional analysis it can be derived that the breakup
time should be of the form:

\[ \tau_{br} = \frac{\mu d}{\sigma} f_\gamma(\lambda) \]  \hspace{1cm} (19)

The function \( f_\gamma(\lambda) \) was correlated to experimental data by Grace (1982) for viscous flows.

**Inertia breakup**

Inertia breakup is found in turbulent flows for droplets larger than the Kolmogorov length scale, \( L_k \). The breakup criterion is formulated in terms of the dimensionless Weber number:

\[ We = \frac{\rho_d \varepsilon^{2/3} d^{5/3}}{2\sigma} \]  \hspace{1cm} (20)

Breakup occurs when \( We \geq We_{cr} \), where \( We_{cr} \) is a function of \( Re_{cr} \), the Reynolds number based on the critical droplet diameter. Furthermore the presence of nearby droplets dampen the disruptive power of the inertia forces, a correction factor containing the volume fraction of droplets is used in the calculation of the critical droplet diameter:

\[ d_{cr} = \left(1 + C_\alpha \alpha \left(\frac{2\sigma We_{cr}}{\rho_c}\right)^{3/5}\right) \varepsilon^{-2/5} \]  \hspace{1cm} (21)

where \( C_\alpha \) is the dispersed phase concentration correction factor.

The value of \( We_{cr} \) is given as function of \( Re_{cr} \):

\[ We_{cr} = 0.069 \frac{Re_{cr}}{Re_{cr}} \]  \hspace{1cm} for \( Re_{cr} < 0.3 \) \hspace{1cm} (22)

\[ We_{cr} = 0.23 \]  \hspace{1cm} for \( Re_{cr} > 0.3 \) \hspace{1cm} (23)

In inertia breakup the breakup time scale follows from the frequency of the second oscillation mode of the droplet:

\[ \tau_{br} = 2\pi k_{br} \left[\left(3\rho_d + 2\rho_c\right)d^3\right] \]  \hspace{1cm} (24)

where \( k_{br} \) is the inertia breakup time constant and \( \rho_d \) is density of the dispersed phase.

**Coalescence model**

The generic form of the coalescence source term is:

\[ s_{cl} = \int_0^\infty \int_0^\infty K_{cl}(d,d')\Delta S^c_\gamma(d,d')n^2P(d)P(d')d(d)d(d') \]  \hspace{1cm} (25)

Similar to the breakup source term, the change in \( S_\gamma \) due to a single coalescence event, \( \Delta S^c_\gamma(d,d') \), can be deduced from the condition of volume conservation during coalescence. Consider two droplets with diameters \( d \) and \( d' \), coalescing together to form a droplet with diameter \( d'' \):

\[ \frac{\pi d^3}{6} + \frac{\pi d'^3}{6} = \frac{\pi d''^3}{6} \Rightarrow d'' = \left(d^3 + d'^3\right)^{1/3} \]  \hspace{1cm} (26)

\[ \Delta S^c_\gamma(d,d') = d'' - (d^\gamma + d'^\gamma) \]  \hspace{1cm} (27)

Since equations (25) and (27) are too complex for efficient computations, the coalescence term is calculated on the basis of a uniform distribution with an equivalent mean diameter, \( d_{eq} \):

\[ \int_0^\infty f(d)n_P(d)d(d) = f(d_{eq})n_{eq} \]  \hspace{1cm} (28)

where \( f(d_{eq}) \) is an arbitrary function of \( d_{eq} \) and:

\[ n_{eq} = \frac{6\alpha}{\pi d_{eq}^3} \]  \hspace{1cm} (29)

The equivalent diameter \( d_{eq} \) is chosen to be proportional to \( d_{sy} \):

\[ d_{eq}(\gamma) = k_{cl,1}d_{sy} \]  \hspace{1cm} (30)

where the proportionality constant \( k_{cl,1} \) is of order unity. Equations (27) and (25) now simplified to:

\[ \Delta S^c_\gamma = d_{eq}^\gamma - \left(d^\gamma + d'^\gamma\right) \]  \hspace{1cm} (31)

\[ s_{cl} = K_{cl}(d_{eq})\Delta S^c_\gamma(d_{eq})n^2_{eq} \]  \hspace{1cm} (32)

\[ = \left(2^{\gamma/3} - 2\right)\left(\frac{6\alpha}{\pi}\right)^2 K_{cl}(d_{eq})d_{eq}^{\gamma-6} \]

\[ \Delta S^c_\gamma = d_{eq}^\gamma - \left(d^\gamma + d'^\gamma\right) \]  \hspace{1cm} (31)

\[ s_{cl} = K_{cl}(d_{eq})\Delta S^c_\gamma(d_{eq})n^2_{eq} \]  \hspace{1cm} (32)

\[ = \left(2^{\gamma/3} - 2\right)\left(\frac{6\alpha}{\pi}\right)^2 K_{cl}(d_{eq})d_{eq}^{\gamma-6} \]
Typically, the coalescence rate $K_{cl}$ is of the form:

$$K_{cl}(d_{eq}) = K_{coll}(d_{eq})P_{coal}(d_{eq})$$

(33)

where $K_{coll}$ is the collision rate, and $P_{coal}$ is the coalescence probability of a single collision event. The collision rate is generally modelled in the form:

$$K_{coll}(d_{eq}) = k_{coll}d_{eq}^2u_{rel}(d_{eq})$$

(34)

where $k_{coll}$ is the collision rate coefficient, and $u_{rel}(d_{eq})$ is the typical velocity difference over a range of $d_{eq}$. The coalescence source term can now be written as:

$$s_{cl} = \left(2^{y/3} - 2\right)\left(\frac{6\alpha}{\pi}\right)^2 k_{coll}u_{rel}(d_{eq})P_{coal}(d_{eq})d_{eq}^{y-4}$$

(35)

### Viscous collision

When two droplets collide they interact for a certain amount of time, forming a dumbbell. During this interaction the film of the continuous phase between the droplets will start to drain. If drainage proceeds down to a certain critical film thickness $h_{cr}$ within the provided interaction time, coalescence will take place; otherwise, the droplets will separate.

For viscous collisions:

$$k_{coll} = \left(\frac{8\pi}{3}\right)^{1/2}$$

(36)

$$u_{rel} = \dot{\gamma}d_{eq}$$

(37)

The coalescence probability is linked to the ratio of the interaction time, $t_i$, and the film drainage time, $t_d$:

$$P_{coal} = \exp\left(-\frac{t_d}{t_i}\right)$$

(38)

The interaction time scale is given by:

$$t_i = \frac{1}{\dot{\gamma}}$$

(39)

The interaction force during the collision is given by:

$$F_i = \frac{3\pi}{2}\mu_i\dot{\gamma}d_{eq}^2$$

(40)

and the critical film thickness is obtained from:

$$h_{cr} = \left(\frac{A_{H}d_{eq}}{24\pi\sigma}\right)^{1/3}$$

(41)

where $A_{H}$ is the Hamaker constant.

### Drainage time

The drainage time scale depends on the mobility of the interface. Four regimes are distinguished:

1. **Fully immobile interface:**

$$t_d = \frac{64\pi\sigma^2 h_{cr}^2}{3\mu_i d_{eq}^2 F_i}$$

(42)

2. **Partially mobile interface (short collision time):**

$$t_d = 3\left(\frac{F_i d_{eq}^2 \sqrt{\mu_d P_d}}{32\pi\sigma^2 h_{cr}}\right)^{2/3}$$

(43)

3. **Partially mobile interface (quasi-steady flow in film):**

$$t_d = \frac{\pi\mu_d \sqrt{F_i}}{2h_{cr}}\left(\frac{d_{eq}}{4\pi\sigma}\right)^{3/2}$$

(44)

4. **Fully mobile interface:**

$$t_d = \frac{3\mu_i d}{4\sigma} \ln\left(\frac{d_{eq}}{8h_{cr}}\right)$$

(45)

### Inertia collision

For inertia collisions:

$$k_{coll} = \left(\frac{2\pi}{15}\right)^{1/2}$$

(46)

$$u_{rel} = (\dot{\gamma}d_{eq})^{1/3}$$

(47)

During inertia collisions, droplet shape oscillations may have a dominant influence on the local approach velocity in the film. In particular the phase difference between the oscillating droplets determines the (local) time of contact, and hence the coalescence probability. Chester (1988) presents an expression for the coalescence probability in such cases:

$$P_{coal} = \frac{\Phi_{max}}{\pi} \left(1 - k_{cl,2}^2 (We - We_0)^2\right)^{1/2}$$

(48)
where $\Phi_{\text{max}}$ is the maximum phase difference and is given by:

$$\Phi_{\text{max}} = \frac{2h_0^3 \rho_0 \sigma}{W_0 \mu_0^2 d_{eq}}$$  \hspace{1cm} (49)

with the following coefficients:

$$k_{c,2} \approx 12.7$$  \hspace{1cm} (50)

$$W_0 \approx 0.8W_{cr}$$  \hspace{1cm} (51)

$$h_0 = 8.3h_{cr}$$  \hspace{1cm} (52)

**Modelling the experiments of Simmons and Azzopardi**

Simmons and Azzopardi (2001) measured droplet size distributions in oil-water flows in a 63mm diameter pipe which was 4.5m long. Kerosene was the continuous phase in the pipe flow, potassium carbonate solution (the dispersed phase and referred as “water” for simplicity) was introduced to the flow through a section of porous pipe wall. The inlet arrangement was designed to minimize the creation of dispersion at the inlet, so that the drops formed were created by turbulence and mixing within the pipe. Two optical methods were used to measure the drop size distribution at the pipe exit.

Many experiments were performed with the pipe in horizontal and vertical positions. One case from the horizontal pipe experiments was selected for analysis by the $S_\gamma$ model described above.

It is important to note that in the experiment the water droplets were introduced to the pipe via perforated holes in the pipe wall. Initially all the drops started close to the pipe wall where turbulence is strongest and the break-up process is also the strongest. To represent this inlet arrangement correctly, the water drops were introduced in a ring close to the pipe wall and an “oil-only” inlet in the pipe centre. This inlet configuration was found to give a fair representation of the distribution profile just downstream of the perforated inlet section in the experiment.

Since the initial drop size at the pipe inlet was not measured and hard to define, several calculations were carried out using different initial drop diameters, 750, 1000 and 1500 microns were used. The computed results for the 1000-micron case are shown below for discussion.

![Figure 1: Dispersed phase volume fraction at pipe exit](image1)

Figure 1 shows the distribution of the water droplets at the pipe exit. It shows clearly that the ring inlet distribution is lost as the droplets travel down the pipe. The droplets are dispersed out from the wall region into the pipe centre mainly by turbulence dispersion, which is modelled by the turbulence dispersion force in STAR-CD. The figure also shows settling effect of the oil droplets. Simmons and Azzopardi made the same observation about droplet settling in their paper.

![Figure 2: Droplet size distribution at pipe exit](image2)

Figure 2 shows a good spread of drop sizes in the pipe exit. The minimum size drops, 155 micron drops, can be found close to the top of the pipe where turbulence and break-up are strongest. The largest size drops, 685 micron drops, are in the centre of the pipe where turbulence and break-up are weakest.
Figure 3: Measured (symbols) and computed (lines) cumulative distribution curves

The measured and computed cumulative distribution curves are shown in Figure 3 above. The comparison only provides an indication of the results obtained, since the measured values were taken at the pipe centre averaged over time, and the computed curves were obtained for the entire cross section at the pipe exit. The comparison suggests that the model slightly under-predicted the amount of small droplets and over-predicted the larger one.

The computational grid used for the current study was in fact quite coarse near the wall, the near wall turbulence was not well resolved. As a result the current model under-predicted the breakup.

The measured curves were obtained at the centre of the pipe exit. Measurements taken from more locations across the pipe cross section would provide a better picture of the droplet distribution across the pipe.

Conclusions

The $S_f$ model described in this paper computes the droplet size distribution based on the method of moment and models for breakup and coalescence. These models were described in detail.

The modelling study shows that it was important to model the experimental set up closely, in this case the inlet arrangement. In the case studied the droplet break-up is the main process. The break-up is mainly caused by the high turbulence in the near wall region. The cumulative drop size distributions show only little dependence on the initial drop diameters. One can expect that the drop size will become independent of initial diameter after passing through a long length of pipe.

The computed results show the expected behaviour of drop dispersion from the wall to the pipe centre and also settling of the drops and more settling for larger diameter drops. The predicted droplet size distribution provided additional useful information about the flow in the pipe.

References


