ADAPTIVE MULTIPLY SIZE GROUP METHOD FOR CFD-Population Balance Modelling of Polydisperse Flows

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INTRODUCTION

Population balance equations (PBE) are the general mathematical framework describing different processes in chemical industry, biotechnology, and environment.[1] Modelling of multiphase multidisperse flows requires a combined CFD-population balance approach. In the past different numerical methods for solution of the population balance equations have been proposed: moving pivot method,[2] method of moments,[3,4] quadrature[5] and direct quadrature[6] method of moments (DQMoM), and the Monte Carlo method.[7-9]

Although these methods and their modifications have been combined with CFD solvers, the problem is far from being resolved. The Monte Carlo method has intrinsic noise, which is not a problem for a spatially homogeneous simulation, but jeopardizes convergence of a CFD solver. The direct quadrature method of moments has an unavoidable stability issue associated with inversion of the Vandermonde matrix.[10] The methods of moments, although providing information about the particle size distribution, do not track any correlation between the particle size and velocity, temperature, etc.

The method of classes,[11,12] also known as the multisize group (MuSiG) method[13] seems the only deterministic method allowing for implementation of an arbitrary coagulation/fragmentation model and accounting for size/velocity interplay. One of the problems that hindered implementation of the method is its computational cost because each size class requires solution of its own momentum and mass balance equations. Since size distribution of the dispersed phase is not known a priori, using a fixed discretisation of the phase space implies that dozens of the size classes should be allocated.

In previous research,[10] we proposed the direct quadrature spanning tree (DQST) method where the discretisation adaptively follows the size distribution. In the present work the univariate version of the DQST method is combined with the STAR-CCM+ simulation software of CD-adapco. In order to underline its affinity with the MuSiG method[13] and the univariate nature of the algorithm (while the DQST is multivariate) the name adopted by CD-adapco for the new feature is the adaptive multisize group (A-MuSiG) method. The A-MuSiG method is implemented in a development version of STAR-CCM+ and will be available for general users in a coming release.

Any model of turbulent flow[14] combines a first principles analysis with empirical modelling. The complex nature of the polydisperse flows implies that even more is postulated rather than analytically derived. In the present study we rely on some first-principles analyses when formulating the Reynolds-averaged transport equations, while the population balance model is postulated without any direct reference to the underlying microscopic models. The article is organized as follows: the Multifluid Model section describes the multifluid approach. The Population Balance Algorithm section provides the details of the A-MuSiG method for univariate population balance problems. The Results and Discussion section contains results of the calculations and demonstrates main features of the method. The paper closes with a brief summary.

MULTIFLUID MODEL

Multiphase fluid dynamics deals with gas-solid (dusty), gas-liquid (sprays), liquid-liquid (emulsions), liquid-solid (suspensions), and liquid-gas (bubbly) flows. Hereafter we refer to the continuous phase (gas, liquid) as “fluid”, while the dispersed phase (particles, droplets, and bubbles) is called “particles”.

In order to account for the multidisperse nature of the flow, the dispersed phase is split into M size groups; from the modelling point of view each group is a separate phase in every aspect but the name. The groups move with their own velocities and exchange mass, momentum, and energy with other groups and with the continuous phase.[13]

Keywords: computational fluid dynamics, fluid mechanics, multi-phase systems, transport processes, fluid-particle dynamics

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The Reynolds-averaged mass conservation equation for the $i$th group reads:
\[
\frac{\partial \rho_p \bar{\alpha}_i}{\partial t} + \nabla \cdot (\rho_p \bar{\alpha}_i \langle u_i \rangle) = m_i - m_y,
\]  
(1)

where $\rho_p$ is the density of the dispersed phase, $\bar{\alpha}_i$ is Reynolds-averaged volume fraction of the $i$th group and $m_i$, $m_y$ are (averaged) mass fluxes from the $j$th group to the $i$th group and from the $i$th group to the $k$th group, respectively; $\langle u_i \rangle$ is phase-averaged velocity of the group:\cite{15}

\[
\langle u_k \rangle_i = \frac{\langle a_i u_k \rangle}{\bar{\alpha}_i},
\]  
(2)

where $a_i$, $u_k$ are instantaneous values of volume fraction and velocity; angular brackets mean Reynolds averaging.

The Reynolds-averaged momentum conservation equation for the $i$th group reads:
\[
\frac{\partial \rho_p \bar{\alpha}_i \langle u_i \rangle}{\partial t} + \nabla \cdot (\rho_p \bar{\alpha}_i \langle u_i \rangle \langle u_i \rangle) = -\nabla p + \nabla \cdot \boldsymbol{\tau}_i + \langle F_i \rangle + m_y \langle u_i \rangle - m_y \langle u_i \rangle,
\]  
(3)

where $\boldsymbol{\tau}_i$ is Reynolds stress and $F_i$ is interaction force between the continuous phase and the $i$th group. The Reynolds stress $\boldsymbol{\tau}_i$ is modelled by a $k-\varepsilon$ model, which can be found elsewhere.\cite{16}

There are different mechanisms responsible for the continuous-dispersed phase interaction: drag, turbulent dispersion, virtual mass, and lift, to name a few. In the present work we assume that for the sake of simplicity that only drag and turbulent dispersion forces (TDF) are important. In the present work we adopt TDF in the Burns et al. form\cite{17} with corrections proposed by Eskin.\cite{18}

Both drag and TDF originate from Reynolds averaging of the instantaneous drag force and are given by the following formulae:
\[
\langle F_i \rangle = \frac{\rho_p}{\tau_{dh}} \bar{\alpha}_i \left( \langle u_i \rangle - \langle u_i \rangle \right) - \frac{\rho_p}{\tau_{dh}} \bar{\alpha}_i D_T \nabla \left( \ln \bar{\alpha}_i - \ln \bar{\alpha}_i \right),
\]  
(4)

where $D_T$ is the coefficient of turbulent dispersion, $\bar{\alpha}_i$ and $\langle u_i \rangle$ are Reynolds-averaged and continuous phase-averaged volume fraction and velocity of the fluid, respectively, and $\tau_{dh}$ is the relaxation time of the $i$th group.

In order to calculate the force (4), the size of the particles in the $i$th group must be specified. Prescribing a constant size for the group one obtains the MuSiG method.\cite{13} If the particle size distribution varies significantly across the system, the fixed discretisation in the size space is not efficient from the numerical point of view. In order to track the size distribution adaptively, Equations (1, 3) must be augmented by an equation for the number density of the $i$th group (strictly speaking, one can formulate an equation for the particles' diameter or some other scalar, but we prefer number density, because of the conservative form of the corresponding equation).

Instantaneous equation for the number density reads:
\[
\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \mathbf{u}_i = S_i,
\]  
(5)

where $S_i$ is the source term due to the breakage and coalescence of the particles. Reynolds averaging of the flux yields:
\[
\langle n_i \mathbf{u}_i \rangle = \bar{n}_i \langle \mathbf{u}_i \rangle + \langle n_i \mathbf{u}_i \rangle.
\]  
(6)

The Reynolds-averaged velocity $\langle \mathbf{u}_i \rangle$ is related to the phase-averaged one as follows:
\[
\langle a_i \mathbf{u}_i \rangle = \bar{\alpha}_i \langle \mathbf{u}_i \rangle = \bar{\alpha}_i \langle \mathbf{u}_i \rangle + \langle a_i \mathbf{u}_i \rangle.
\]  
(7)

Therefore
\[
\langle \mathbf{u}_i \rangle = \langle \mathbf{u}_i \rangle - \frac{\langle a_i \mathbf{u}_i \rangle}{\bar{\alpha}_i}
\]  
(8)

and using the gradient hypothesis
\[
\langle n_i \mathbf{u}_i \rangle = -D_T \nabla \bar{n}_i, \quad \langle a_i \mathbf{u}_i \rangle = -D_T \nabla \bar{\alpha}_i
\]  
(9)

the Reynolds-averaged Equation (5) can be written in the following form:
\[
\frac{\partial \bar{n}_i}{\partial t} + \nabla \cdot \bar{n}_i \left( \langle \mathbf{u}_i \rangle + D_T \nabla \left( \ln \bar{\alpha}_i - \ln \bar{n}_i \right) \right) = \langle S_i \rangle.
\]  
(10)

Note that if the group's volume $\bar{\alpha}_i / \bar{n}_i$ is constant $\nabla \ln \bar{\alpha}_i - \ln \bar{n}_i = 0$ and the diffusive velocity in Equation (10) vanishes. In the present work we employ Equation (10) in a more convenient form:
\[
\frac{\partial \bar{n}_i}{\partial t} + \nabla \cdot \bar{n}_i \left( \langle \mathbf{u}_i \rangle + D_T \nabla \ln \bar{\alpha}_i \right) - \nabla \cdot D_T \nabla \bar{n}_i = \langle S_i \rangle.
\]  
(11)

Having the mean volume fraction and number density, one can postulate the volume of the particles in the $i$th group as
\[
\bar{v}_i = \frac{\bar{\alpha}_i}{\bar{n}_i}.
\]  
(12)

Note that $\bar{v}_i$ is not equal to the Reynolds-averaged volume of the group $\langle v_i \rangle$, i.e., averaging of the instantaneous values of the volume fraction, number density and group's volume yields:
\[
\bar{\alpha}_i = \langle v_i n_i \rangle = \bar{n}_i \bar{v}_i = \bar{n}_i \langle v_i \rangle + \langle n_i v'_i \rangle
\]  
(13)

and two averaged volumes are related via the following equation:
\[
\bar{v}_i = \langle v_i \rangle + \frac{\langle n_i v'_i \rangle}{\bar{n}_i}.
\]  
(14)

The correlation in (14) can be estimated using the gradient hypothesis as follows:
\[
\langle n_i v'_i \rangle = \bar{l}_T^2 \nabla \bar{n}_i \cdot \nabla \langle v_i \rangle
\]  
(15)

where $\bar{l}_T$ is a turbulent length. Combining Equations (14–15) one obtains:
\[
\frac{\bar{v}_i}{\langle v_i \rangle} = 1 + \bar{l}_T^2 \nabla \ln \bar{n}_i \cdot \nabla \ln \langle v_i \rangle
\]  
(16)

Since it is unlikely that $\bar{v}_i$ and $\langle v_i \rangle$ vary by an order of magnitude at the distance $\bar{l}_T$, the last term in Equation (16) can be neglected; hereafter we assume that $\bar{v}_i = \langle v_i \rangle$.

Being similar to the DQMoM method, the A-MuSiG method suffers from so-called spurious dissipation,\cite{6,19} i.e., the turbulent
dispersion leads to an underestimation of the standard deviation of the particle size distribution. To amend this effect an additional term has to be added to the RHS of (11). In the present work we neglect this term for the sake of numerical efficiency assuming that it is negligible in comparison to coalescence and breakage.

**POPULATION BALANCE ALGORITHM**

In order to close the model described by amending Equations (1, 3, 11, 12) one must specify \( m_{ij}, m_{ik} \) and \( \langle S_i \rangle \); this is done with a population balance algorithm. Note that the population balance algorithm is local; that is, in the present section we ignore the spatial variations of the parameters of interest and concentrate on a single cell of a finite volume method.

The A-MuSiG method consists of two key elements:\cite{10}

- Assume that a particle of size \( \nu' \) is created as a result of either coalescence or breakup. Since \( \nu' \) is not equal to any \( \nu_i \) number densities and volume fractions of the newly created particle must be redistributed among the existing groups.
- Initially, each group has the same volume fraction; as a result of coalescence, breakup, and transport some groups gain mass, while others lose it. In order to restore the equal distribution of \( \nu_i \) among the groups we use a smoothing procedure.

**Preliminary Considerations: Dealing With a Newly Created Particle**

Let us arrange the groups by their size: \( \nu_1 < \nu_2 < \ldots \nu_M \). We say that if \( \nu_i \leq \nu' \leq \nu_{i+1} \), the newly created particle belongs to the \( (\nu_i, \nu_{i+1}) \) pair of groups; if \( \nu_M \leq \nu' \) it belongs to the \( (\nu_M, \nu_{M+1}) \) pair; if \( \nu' \leq \nu_1 \) it belongs to the \( (\nu_1, \nu_2) \) pair. Applying the DQMO method to the chosen pair and demanding that the zero, first, and second moments of the particle size distribution are conserved (for details see Appendix A), one obtains the following system of equations:\cite{6, 10}

\[
\begin{align*}
\frac{dW_1 + dW_2}{dP_1 + dP_2} &= 1, \\
-\nu_i^2 dW_1 + 2\nu_i dP_1 - \nu_{i+1}^2 dW_2 + 2\nu_{i+1} dP_2 &= \nu'^{2},
\end{align*}
\]

where vector \([dW_1, dP_1, dW_2, dP_2] \) contains the increments of \( \nu_i, \nu_i, \nu_{i+1}, \) and \( \nu_{i+1} \) due to addition of a single particle of size \( \nu' \). The solution of Equation (17) reads:

\[
\begin{align*}
W_1 &= \mu, \\
W_2 &= 1 - \mu, \\
P_1 &= \nu' - dP_1, \\
P_2 &= \mu (\nu_i + \nu_{i+1}) + \frac{r^2}{2}(\nu_i - \nu_{i+1}),
\end{align*}
\]

where \( r = \frac{\nu_{i+1} - \nu'}{\nu_{i+1} - \nu_i} \) and \( \mu \) is a free parameter. In the present work \( \mu \) is specified as follows:

\[
\mu = \begin{cases} 
(2 - r)r &: r \leq 0, \\
r &: 0 \leq r \leq 1, \\
r^2 &: 1 \leq r.
\end{cases}
\]

This choice of \( \mu \) ensures that \( d\nu_i(\nu' - \nu_i) \geq 0 \), i.e., the group’s size moves toward \( \nu' \) and not in the opposite direction.

![Figure 1. Counter-gravity flow: \( L_2 \) error of \( d_{32} \) for different \( M \); the dashed line has slope \(-1.5\).](image)

**Physical Processes: Coagulation and Breakup**

Using the algorithm described by Equations (17–19) one can solve the population balance problem as follows.

**Coagulation**

Rate of the coagulation between \( k^{th} \) and \( l^{th} \) particles is

\[
R_{kl} = \left( 1 - \frac{1}{2} \delta_{kl} \right) K(\nu_k, \nu_l)\nu_i\nu_i.
\]

where \( K(\nu_k, \nu_l) \) is a coagulation kernel and the term with Kronecker delta aims to prevent double counting of coagulation of two equal particles. A new particle of size \( \nu' = \nu_k + \nu_l \) is formed and it has to be assigned to its nearest pair \( (\nu_i, \nu_{i+1}) \) as it is described in the previous section and for each coagulation event the coefficients \( m_{pq} \) and \( \langle S_p \rangle \) are updated as follows:

\[
\langle S_k \rangle := \langle S_k \rangle - R_{kl}, \\
\langle S_l \rangle := \langle S_l \rangle - R_{kl}, \\
\langle S_i \rangle := \langle S_i \rangle + \mu_k R_{kl}, \\
\langle S_{i+1} \rangle := \langle S_{i+1} \rangle + (1 - \mu_k)R_{kl}.
\]

\[
m_{ik} := m_{ik} + \rho_p R_{kl} \nu_i dP_1, \\
m_{il} := m_{il} + \rho_p R_{kl} \nu_l dP_1, \\
m_{(i+1)k} := m_{(i+1)k} + \rho_p R_{kl} \nu_k dP_2, \\
m_{(i+1)l} := m_{(i+1)l} + \rho_p R_{kl} \nu_l dP_2.
\]

**Breakup**

Breakup of the particles is characterised by two functions: breakup rate \( b(\nu_k) \) and daughter particle distribution \( P(\nu_k|\nu') \).\cite{1} In the present work we approximate \( P(\nu_k|\nu') \) by a discrete measure:

\[
P(\nu_k|\nu') \approx \sum_{j=1}^{M} w_j(\nu_k)\delta(\nu' - \nu_j(\nu_k)).
\]

The rate of creation of of particles of size \( \nu_i \) due to the breakage of \( \nu_k \) particles is

\[
h_{kj} = b(\nu_k)w_j(\nu_k)\nu_k.
\]

The particle is assigned to its nearest pair \( (\nu_i, \nu_{i+1}) \) according to Equations (17–19) and the coefficients \( m_{pq} \) and \( \langle S_p \rangle \) are updated.
as follows:

\[
\langle S_k \rangle := \langle S_k \rangle - h_{kj}, \\
\langle S_i \rangle := \langle S_i \rangle + \mu_i h_{ij}, \\
\langle S_{i+1} \rangle := \langle S_{i+1} \rangle + (1 - \mu_i) h_{kj}.
\] (25)

\[
m_{ik} := m_{ik} + \rho_t h_{kj} \nu_k dP_1, \\
m_{(i+1)k} := m_{(i+1)k} + \rho_t h_{kj} \nu_k dP_2.
\] (26)

Breakup and coalescence are the two most prominent examples of particle creation/disappearance; other terms of the population balance equation (inlet boundary conditions, nucleation, etc.) can be implemented in the same way.

Final Step: Volume Fraction Smoothing

During time interval \(dt\) the volume fractions of the groups changes as:

\[
\sigma_i' = \sigma_i' + \frac{dt}{\rho_p} \sum_{i=1}^{M} (m_q - m_p).
\] (27)

In order to restore the equal distribution of the volume fractions among the groups we make use of Equation (18).

Denote the free parameter \(\mu\) belonging to the \((\sigma_i, \sigma_{i+1})\) pair as \(\mu_i\). It follows from Equation (18) that if number densities and volume fractions are updated according to the following formulæ:

\[
\pi_i = \pi_i + \mu_i - \mu_{i-1}, \\
\bar{\sigma}_i = \bar{\sigma}_i + \frac{1}{2} (\bar{\sigma}_{i+1} + \bar{\sigma}_i) \mu_i - \frac{1}{2} (\bar{\sigma}_{i-1} + \bar{\sigma}_i) \mu_{i-1},
\] (28)

where the first three moments of the particles size distribution are unchanged for any \((\sigma_i, \sigma_{i+1})\) pair;\(^{10}\) in Equation (28) we assume that \(\mu_0 = \mu_M = 0\). Requiring that \(\bar{\sigma}_1 = \bar{\sigma}_2 = \ldots = \bar{\sigma}_M\) one obtains the following minimization problem:

\[
\bar{\mu} = \arg \min_{\mu} \left\{ \frac{1}{2} \sum_{i=1}^{M-1} \left[ \bar{\sigma}_i + \frac{1}{2} (\bar{\sigma}_{i+1} + \bar{\sigma}_i) \mu_i - \frac{1}{2} (\bar{\sigma}_{i-1} + \bar{\sigma}_i) \mu_{i-1} \right]^2 \right\}.
\] (29)

Differentiation of the above equation with respect to \(\mu_i\) yields a linear algebraic equation with three-diagonal matrix:

\[
a_i \mu_{i-1} + b_i \mu_i + c_i \mu_{i+1} = d_i,
\] (30)

\[\text{Figure 2. Flow through an orifice; flow field (a) and mean breakage rate (b).}\]

\[\text{Figure 3. Flow through an orifice: group diameters (a), volume fraction (b) and d}_{32} (c) calculated with 7 (circles) and 3 (crosses) groups; the upper line is for U}_{in} = 0.2 m/s and the lower is for U}_{in} = 0.4 m/s.}\]
Figure 4. Bubbly flow through a horizontal pipe: velocity of the smallest (a), medium-size (b), and biggest (c) bubbles; \( \theta_{in} = 4 \text{ m/s}, \omega_{in} = 0.1 \).

where

\[
\begin{align*}
  a_i &= -(\bar{v}_{i-1} + \bar{v}_i), \\
  b_i &= 2(\bar{v}_{i+1} + \bar{v}_i), \\
  c_i &= -(\bar{v}_{i+1} + \bar{v}_{i-1}), \\
  d_i &= 2(\bar{v}_{i+1} - \bar{v}_i), \\
  a_0 &= c_{M-1} = 0.
\end{align*}
\tag{31}
\]

Once Equation (30) is solved, the coefficients \( m_{pq} \) and \( \langle S_q \rangle \) are updated as follows:

\[
\begin{align*}
  \langle S_i \rangle &= \langle S_i \rangle + \mu_i - \mu_{i-1}, \\
  m_{i(i-1)} &= m_{i(i-1)} + \frac{\rho \rho}{2} \max(\mu_{i-1}, 0)(\bar{v}_{i-1} + \bar{v})_i, \\
  m_{i(i-1)i} &= m_{i(i-1)i} - \frac{\rho \rho}{2} \min(\mu_{i-1}, 0)(\bar{v}_{i-1} + \bar{v}_i) \tag{32}.
\end{align*}
\]

RESULTS AND DISCUSSION

Counter-Gravity Flow

Since Equation (17) ensures conservation of the first three moments of the distribution (zeroth, first, and second), one might expect that the population balance equations are solved with second-order accuracy with respect to \( M \). In order to test precision of the A-MuSiG method, i.e., combination of the population balance with transport equations, we performed the following numerical test. Small solid particles (\( d = 10^{-5} \text{ m} \)) are blown up by air in a 10 m long pipe against gravity and coagulate with size-independent rate (\( K(\bar{v}_k, \bar{v}_l) = \text{const} \)); velocity of air is 5 m/s. As a result of coagulation the particles grow, so the settling velocity at the outlet varies from 0.5 m/s for the smallest particles to 4.5 m/s for the largest ones. We performed calculations with different \( M \) from 3 to 128. Regarding the solution with the highest \( M \) as exact we have computed \( L_2 \)-norm error for the Sauter mean diameter \( d_{32} \). The results are presented in Figure 1; in this case the overall accuracy of the A-MuSiG method is between first and second order.

Flow Through an Orifice

Although the convergence rate at \( M \to \infty \) provides an indication of precision of the method, our focus is on accuracy with a small (\( M \approx 3 - 7 \)) number of groups. Flow through an orifice is widely used for investigation of breakup processes in two-phase systems. We model flow through a 3 cm diameter pipe obstructed by a 1.5 cm diameter orifice under conditions similar to Galinat et al. We performed calculations with different \( M \) from 3 to 128. Regarding the solution with the highest \( M \) as exact we have computed \( L_2 \)-norm error for the Sauter mean diameter \( d_{32} \). The results are presented in Figure 1; in this case the overall accuracy of the A-MuSiG method is between first and second order.

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Martínez-Bazán et al. the process is governed by the competition between the capillary forces and dynamic pressure of the turbulent flowfield. The most intensive turbulence is generated in the mixing layer between the jet and the recirculating flow. It is where the mean breakage rate:

$\langle b \rangle = \frac{\sum b(v_i)n_i}{\sum n_i}$

attains its maximum. The results are in qualitative agreement with the experimental observations. The adaptive nature of the method is illustrated in Figure 3: starting with a narrow size distribution one obtains a much wider distribution of small droplets. It is clear that a constant discretisation of the phase space would require a much larger number of the size groups. As one can see, the Sauter mean diameter calculated with 3 groups is nearly identical to the predictions obtained with 7 groups. The small bump in $d_{32}$ is due to the acceleration and subsequent deceleration of the flow. Since the dispersed phase has lower density, the smaller droplets decelerate more slowly and therefore increase the percentage of bigger droplets in the deceleration zone behind the obstacle. Due to the volume fraction smoothing procedure the volume fractions of all groups remain equal, although they vary along the pipe. The higher volume fraction of the dispersed phase behind the orifice is due to the breakage and consequent decrease of the interphase slip velocity.

Bubbly Flow in a Horizontal Pipe

Bubbly flow in a horizontal pipe similar to that studied experimentally by Andreussi et al. is a good illustration of the advantages of the A-MuSiG method. We model gas-liquid flow through a 5 cm diameter pipe; coalescence and breakup of the bubbles is modelled using Luo’s and Martínez-Bazán et al.’s models, respectively. Velocity at the inlet and volume fraction of the gas phase at the inlet are $U_{in}$ and $\alpha_{in}$. The pipe is 20 m long and we are interested in the flow patterns far away from the inlet where the transient effects are negligible. Results of the calculations are presented in Figures 4–5.

Although a size group isn’t a physical reality, but a numerical construct aiming to model the polydisperse flow, it is instructive to inspect velocity plots of different groups. Vertical stratification of the flow is governed by balance of two forces: the buoyancy force driving the bubbles up and the TDF pushing them down. However, relative strength of these forces depends on a bubble’s size, that is, the bigger the bubble stronger the buoyancy. As one can see, there is a permanent countercurrent of bubbles with different sizes: big bubbles rise up, where they are broken, while small ones flow down and coalesce.

Elrerin et al. investigated scavenging of atmospheric pollutants by falling rain droplets and discovered that the difference in settling velocities $U_s$ results in the effective pseudo-diffusion coefficient

$D = \tau_{rel} \langle (U_t - U_s)^2 \rangle,$

where $\tau_{rel}$ is a relaxation time. In the current circumstances it is conceivable to estimate $\tau_{rel}$ as the mean time between consecutive breakage/coalescence events, experienced by a single bubble. Using the mean breakup and coalescence rates one obtains:

$\tau_{rel} \approx \frac{\langle b \rangle}{\langle b \rangle + 2 \langle R \rangle}.$
where \( \langle n \rangle \) is the total number density of the bubbles and the coefficient 2 in front of the coalescence rate is because a coalescence event involves two bubbles. The ratio of the obtained pseudo-diffusivity (viscosity) to the turbulent viscosity \( \nu_T \) is presented in Figure 5c. As one can see, the pseudo-viscosity ratio is of order one; that is, considering different velocities for different size classes significantly alters predicted momentum, heat, and mass transfer across the pipe. Unlike previously published CFD-population balance models (see, e.g., Ekambara et al.\cite{26}) the A-MuSiG method does not assume a common velocity for all size groups and therefore provides a more detailed description of the transport process.

Accuracy of the method is well-characterised by the results presented in Figure 6. As one can see, the Sauter mean diameter predicted with \( M = 3 \) is quite close to that calculated with \( M = 7 \). Note that the A-MuSiG method is rather expensive computationally: using three size groups approximately doubles the required CPU time in comparison to a two-phase flow; \( M = 5 \) triples it, etc. Since STAR-CCM+ is an iterative solver, we start our calculations with the minimum possible number of size groups (3) and after getting a converged solution \( M \) was increased gradually.

An Agitated Tank

Flow patterns and size distribution of the dispersed phase in an agitated tank have been the subject of numerous experimental, theoretical, and numerical works (see, e.g., Pacek et al.\cite{27} and references therein). Although detailed consideration of the problem is outside of the scope of the present paper, we created a “toy” model of an agitated tank as shown in Figure 7. It is a cylindrical vessel with 8 baffles and an 8-blade impeller. Since we neglect the effects of gravity, only \( \frac{1}{16} \) of the physical domain has to be modelled. In our computations angular velocity of the impeller varies from 150 rpm to 450 rpm; the continuous phase is water, while densities of the dispersed phases vary from 850 \( \text{kg/m}^3 \) to 1050 \( \text{kg/m}^3 \).

After a transient period the breakup and coalescence reach a dynamic equilibrium; breakup is more intensive near the baffles (where the turbulent dissipation rate is maximum), while coalescence is more uniformly distributed across the system. Due to intensive recirculation the variation in droplet diameter is quite small, which is why other parameters have been chosen to verify accuracy of the method; Figure 8 shows breakup and coalescence rates along a radius (intersection of two symmetry planes shown in Figure 7) predicted with different numbers of the size groups. The spread of the results is higher than in the previous tests, but one has to remember that these characteristics are more sensitive than mean diameter, i.e., coalescence and breakup contribute to time derivative of a particle’s size.

CONCLUSIONS

1. A framework for combined PBE-CFD modelling of polidisperse multiphase flows is proposed.
2. The dispersed phase is represented as a set of size groups interacting via the population balance algorithm.
3. Each size group has its own number density, mass, and momentum balance.
4. The A-MuSiG method is adaptive, that is, the size of each group is not a prescribed constant, but is a part of the solution.
5. The adaptivity is enforced via the condition that in each cell every size group accounts for the same portion of the total mass and each group has equal contribution to the system’s dynamics. Therefore, computational resources are allocated more efficiently.
6. Since the A-MuSiG method only requires solution of a tridiagonal diagonally-dominant equation, it is robust for any number of size groups.
7. Due to the adaptive nature of the method, only a small number of size groups are needed to estimate mean size, interfacial area, and other characteristics of interest.

NOMENCLATURE

Greek Symbols

\( \alpha \) \hspace{1em} \text{volume fraction}
\( \rho \) \hspace{1em} \text{density}

Roman Symbols

\( b \) \hspace{1em} \text{breakage rate}
\( K \) \hspace{1em} \text{coagulation kernel}
\( m \) \hspace{1em} \text{mass transfer rate between the size groups}
\( n \) \hspace{1em} \text{number density}
\( P \) \hspace{1em} \text{daughter particles distribution}
\( S \) \hspace{1em} \text{source term of the number density equation}
\( u \) \hspace{1em} \text{velocity}
\( v \) \hspace{1em} \text{volume of a particle}

Subscripts

\( f \) \hspace{1em} \text{fluid}
\( i \) \hspace{1em} \text{\( i \)th size group}
\( p \) \hspace{1em} \text{particles}

APPENDIX A

In the DQMoM method we look for the solution of a spatially homogeneous version of Equation (5) in the following form\cite{19,6,10}

Figure 8. Breakup and coalescence in agitated tank calculated with 3 (circles), 5 (diamonds), and 7 (triangles) groups.
(hereafter we adopt the notations used in Fox[19]):

\[
n(t, x) \approx \sum_{i=1}^{M} w_i(t) \delta(x - x_i(t)), \tag{A1}
\]

where \(\delta(x)\) is the Dirac delta function. The abscissae \(x_i\) represent “computational particles”, that is each abscissa represents \(w_i\) physical particles with identical properties.

Substitution of the above equation into the LHS of Equation (5) yields:

\[
\frac{dw_i}{dt} \delta(x - x_i) - \frac{dx_i}{dt} \cdot \delta(x - x_i) = \frac{dw_i}{dt} \left( \delta(x - x_i) + x_i \cdot \delta'(x - x_i) \right) - \frac{dw_i}{dt} \cdot \delta'(x - x_i). \tag{A2}
\]

where \(\delta'(x)\) is derivative of Dirac delta function. Denoting the weighted abscissas as \(p_i = w_i x_i\) one obtains the following unclosed form of Equation (5):

\[
\sum_{i=1}^{M} \left( \frac{dw_i}{dt} \left( \delta(x - x_i) + x_i \cdot \delta'(x - x_i) \right) - \frac{dp_i}{dt} \cdot \delta'(x - x_i) \right) = S(n(t, x)). \tag{A3}
\]

In order to close Equation (A3) we successively multiply it by linearly independent polynomials and integrate by \(x\). In the monovariate case any \(2M\) polynomials \(H_i(x)\), \(i = 1, 2, \ldots 2M\) of order \(2M - 1\) yield equivalent (up to a linear transformation) systems of ordinary differential equations with respect to \(w_i\) and \(p_i\):

\[
\begin{bmatrix}
\frac{dw_1}{dt} \\
\frac{dp_1}{dt} \\
\vdots \\
\frac{dw_M}{dt} \\
\frac{dp_M}{dt}
\end{bmatrix} = \int_{0}^{\infty} \begin{bmatrix}
H_1(x) \\
H_2(x) \\
\vdots \\
H_{2M}(x)
\end{bmatrix} L(n(x)) dx, \tag{A4}
\]

where

\[
\begin{align*}
A_{ij,2j-1} &= H_i(x_j) - x_j H'_i(x_j), \\
A_{ij,2j} &= H'_i(x_j), \\
i &= 1, \ldots 2M, \\
j &= 1, \ldots M. \tag{A5}
\end{align*}
\]

Using only two abscissae \((M = 2)\) and three polynomials \((H_i(x) = 1, x, x^2)\) one obtains for \(A\):

\[
A = \begin{bmatrix}
1 & 0 & 1 \\
0 & 0 & 1 \\
-x_1^2 & 2x_1 & -x_2^2 & 2x_2
\end{bmatrix} \tag{A6}
\]

REFERENCES