Simulation methods for polydisperse, multiphase flows using moment methods

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Simulation methods for polydisperse, multiphase flows using moment methods

by

Jeffrey C. Heylmun

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

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The student author, whose presentation of the scholarship herein was approved by the program of study committee, is solely responsible for the content of this dissertation. The Graduate College will ensure this dissertation is globally accessible and will not permit alterations after a degree is conferred.

Iowa State University
Ames, Iowa
2019

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DEDICATION

This thesis is dedicated to my wife Katie, and to my family and friends who supported me throughout the journey they call graduate school.
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ABSTRACT

While the ability to solve for multiphase flows that contain a distribution of properties is crucial to the accurate prediction of physical system, there is currently a lack of numerical solution methods to solve for these types of flows. In this work, three new numerical procedures are developed in order to accurately solve for systems containing polydisperse multiphase flows, and flows with velocity distributions. The ability to correctly solve these flows allows for the local segregation of size that is generally not possible due to the limitations of the standard solution techniques. First, a numerical algorithm is presented to solve bubbly flows using the standard two fluid model coupled to the moment transport equations of a monokinetic number density function (NDF). This provides the stability of a two-fluid solver, while adding additional accuracy that comes from the inclusions of a range of sizes, and corresponding velocities. The algorithm is first tested to ensure numerical stability, and then validated against experimental data, as well as the two-fluid and multi-fluid models. Next, a semi-implicit solution method for the handling of the particle pressure flux for polydisperse granular systems is presented in the multifluid framework, and is based on the work of Syamlal et al. (1993). The method is first verified by examining the segregation of sizes in a settling bed, then is validated against existing implementations of polydisperse kinetic theory, as well as experimental results in a bidisperse fluidised bed and a cyclic vertical riser. Finally, a solution method to the transport of the joint size-velocity NDF is presented using QBMM. The presented method makes no assumptions on the size or velocity distribution. Additionally, the relevant source terms to describe change in size are presented using a volume fraction formulation. This becomes very important for numerical stability when small particles are under consideration. The solution procedure is first validated using simple 0-D cases for both population balance equations and collision models. A collection of 1-D axisymmetric spray cases are then used to validated both the joint size-velocity distribution evolution. Finally a set of 2-D
crossing jet cases are presented to show the ability of the method to account for multiple velocities within a single cell. All work has been implemented in the open-source framework OpenFOAM.
CHAPTER 1. INTRODUCTION

Multiphase flows can be seen in a wide range of industries, from grain transport and storage to nuclear power plants and coal combustion. While multiphase systems are extremely common in industry, the study of simulation methods to accurately predict characteristics of the flows is an ongoing topic of investigation. The ability to correctly describe physical, complex systems allows for improvements in both production quality as well as efficiency of processes. There are three main types of multiphase flows that will be the focus of this work: particulate flows, bubbly flows, and flows with droplets. The first consists of fluidized bed reactors used in petroleum refinement and coal combustion, particle mixing in bio-oil production (Ringer et al., 2006), grain and powder transport and storage (Harnby, 1992), sediment transport in oil pipelines (Shirazi et al., 2015), and chemical processes such as flash-nano precipitation (Cheng et al., 2010). Bubbly flows are commonly seen in nuclear power generation for the cooling of reactors due to high rates of heat transfer (Ho et al., 2008; Yeoh and Tu, 2006), and in the processing of chemicals due to the high rates of mass transfer (Shah et al., 1982), both due to the high surface area between the gas and liquid phases. Lastly, droplets (or sprays) are used in combustion processes (Laurent and Massot, 2001) and in production of metal powders (Hernandez et al., 2019). The main difficulties in simulating these flows come about due to the fact that the amount of information required to solve the entire system is often far large to be tractable. Typically there are assumptions made about the underlying statistics of the flow, such as only the mean quantities are important, which allow for a reduction in the computational cost. This will be the focus of this work, specifically cases with a wide size distribution, and systems in which the Knudsen number is high resulting in a distribution of velocities which is not Maxwellian.
The mathematical description of all these processes is necessary to be able to accurately predict the flow patterns. Currently there exist a lack of solution techniques to efficiently handle a distribution of properties in a small control volume (such as polydisperse systems) in an efficient manner. As an example of why this is important, when flows have a wide distribution of sizes at a given spatial location, momentum exchange terms between phases tend to result in segregation of sizes primarily due to the drag and lift forces. Both of these forces are driven by the slip velocity between the dispersed and continuous phases which can vary within a cell in which a distribution of forces is present. Additionally when a distribution of velocities is present, this also leads to the addition of terms to account for deviations of velocities from the mean. The two-fluid model (Drew and Lahey, 1987), which is typically the model of choice to solve most two-phase or multiphase systems, considers only mean quantities (diameter, velocity), and therefore the ability for different sizes to segregate due to forces within a control volume becomes impossible to predict. Due to the range of Stokes number present in multiphase flows, different degrees of approximations can be made to simplify the solution procedure and reduce the computation cost. This can range from non-inertial particles (St = 0) where the particles exactly follow the fluid streamlines, to monokinetic particles or bubbles in which each size corresponds to a unique velocity, to inertial particles (St \( \gg 1 \)) in which a single particle size can have a distribution of velocities. These will all be discussed in more detail below.

### 1.1 Number density description

In order to keep a cohesive description of the methods used to solve multiphase problems, the number density function (NDF) of a particle population will be introduced. The behavior of a dispersed phase can be completely described by the evolution equation for a joint size-velocity NDF, where \( f(t, x, \xi, v) \) is the NDF, and is dependent on time, position, particle size, and particle velocity, denoted as \( t, x, \xi, v \), respectively. The transport equation for the NDF is given by:

\[
\frac{\partial f}{\partial t} + \nabla_x \cdot (fv) + \nabla_\xi \left[ G(\xi)f \right] + \nabla_v \cdot \left\{ [A(\xi, v) + g] f \right\} = C,
\] (1.1)
where $\nabla_x \cdot (f v)$ represents the advection of the NDF in physical space, $\nabla_\xi \cdot [G(\xi) f]$ is the advection term in coordinate space and represents growth, $\nabla_v \cdot \{ [A(\xi, v) + g] f \}$ represents the change in the velocity components of the NDF due to external accelerations or forces such as drag ($A$) and gravitational acceleration ($g$), and $C$ is the change due to collision between particles (aggregation, breakup, etc.).

The complete form of this equation is for a $(1+3+1+3)N$ $(8xN)$ dimensional distribution (one time, three space, one size, three velocity, and N particles dimensions). This results in a distribution where each particle has its own NDF, dependent on every other particle position, size, and velocity. Obviously this becomes intractable for systems with a large number of particles when the individual particles are not used to evolve the NDF evolution equation. To simplify the distribution, all particle distributions are assumed to be independent and identical to one another, leading to the assumption that one size-velocity distribution can be used describe that of every particle. Further simplifications of the distribution can be made by means of the Stokes number, where the Stokes number is defined as the ratio of particle response time (drag time) to that of the surrounding fluid’s time scale. A Stokes number of zero corresponds to a collection of particles that exactly follow the streamlines of the surrounding fluid, while a Stokes number of infinity correspond to a collection of particles that is not influenced by the surrounding fluid. The prior, results in a distribution that can be described using a 1-D or univariate size distribution (Ramkrishna, 2000). These types of distributions will change due to aggregation, breakup, growth, and nucleation sources that occur either due to particle-particle interactions, or fluid-particle interactions. Flows which satisfy the univariate simplification are most commonly seen in the chemical engineering industry where small particles are grown, such as in a Taylor-Couette reactors (Marchisio et al., 2003), or in chemical mixing processes where the statistics of composition are considered in place of those of size (Fox, 2003).

Once particles are able to deviate the continuous phase streamlines due to non-zero Stokes numbers, momentum transfer occurs between the dispersed and continuous phases, and can be important in describing the evolution of both phases depending on mass loading and volume fraction.
When the mass loading/volume fraction is sufficiently low, an assumption of one-way coupling can be made where the dispersed phase is affected by the fluid, but the fluid is not affected by the dispersed phase. For higher mass loading, the influence of the momentum transfer between phases will cause changes in the continuous phase momentum. When the volume fraction is sufficiently high, the volume occupied by the dispersed phase must be accounted for in the conservation equations of the fluid. These last two cases will be considered two-way coupling. The main source of momentum transfer comes from drag, however lift, virtual mass, and wall lubrication can also be important depending on the particle size, relative velocity, density ratio, etc. These forces are highly dependent on the particle size as well as the slip velocity between phases, and will change both phases' flows characteristics in non-trivial ways. Correctly accounting for polydispersity and variations in velocity is then essential to accurately predicting the forces and therefore the entire evolution of the multiphase system.

Particles with a non-zero Stokes number, but less than order one will see variations in velocity due to size. This results in the monokinetic assumption (Laurent and Massot, 2001) in which the drag time is fast enough that all particles of a given size have a negligible velocity variance, but a size conditioned mean velocity. This type of flow is most common with bubbly flows and other low density particulate flows. This approximation allows for segregation of sizes which can occur due to drag, lift, and other momentum exchange terms, while greatly reducing the computational cost in comparison with the joint size-velocity NDF evolution.

Once the Stokes number of a particle is greater than order one, the variance of velocity as well as other higher order statistics can become important. This deviation from a velocity delta distribution leads to the possibility of particle-particle collisions in more dense regimes, and particle trajectory crossing (PTC) in dilute regimes. In comparison with flows with univariate or even monokinetic distributions, these flows tend to be much more chaotic in nature due to the fact that particle streamlines can cross within a computational cell. The interactions of particles through collisions and PTC lead to a non-Maxwellian VDFs, meaning that higher order statistics must be considered to accurately track the NDF evolution. This is illustrated in the solution of the particle velocity
distribution in Taylor-Green vorticies at varying Stokes numbers (Desjardins et al., 2008; Yuan and Fox, 2011).

1.2 Existing methods

There are two types of methods for describing the evolution of a collection of discrete entities, either the collection of dispersed phase entities are individually tracked and evolved to obtain a single realization of the flow, or continuous statistical quantities of distribution are evolved to predict the overall shape of the distribution for all realizations of the flow.

1.2.1 Single realization methods

Single realization methods are often used to describe relatively small collection of elements due to the fact that they tend to be far too expensive to describe real, large scale systems. From a theoretical point of view they also tend to be simple, due to the fact that they describe the evolution of fluid and particles using only the fundamental evolution equations. This removes the need for models, and instead these methods are often used to develop models that can then be used in the statistics based models.

For a dispersed phase that is assumed to have a constant, spherical shape, Lagrangian particles are used to represent the discrete entities. This allows the evolution of the distribution to evolve due to elements with unique velocities as well as collisions. This method is typically applied to particulate flows for DNS simulations with using the immersed boundary method (Peskin, 1982; Tenneti et al., 2011) where the flow is fully resolved around every particle. The Euler-Lagrange method is used for meso-scale simulations where the flow is not fully resolved around every particles so models are used for drag and other sources of momentum transfer. This removes the need to use KTGF to model the transport properties of a granular phase, and includes the ability to capture multi-point phenomena such as clustering (Capecelatro and Desjardins, 2013) that is hard to capture with statistical modeling. While the Euler-Lagrange method is typically used for particulate flows, it also is used for both bubbly flows (Sokolichin and Eigenberger, 1994) and
droplets (Laurent and Massot, 2001), with the assumption that the bubbles or droplets are spherical with non-changing shape.

When the shape of the dispersed phase population becomes important, alternative methods must be used. Methods such as the volume of fluid (Noh and Woodward, 1976; Youngs, 1982), level-set (Osher and Sethian, 1988), or interface tracking (Unverdi and Tryggvason, 1992) approximate the curvature of the interface between the phases so that the surface tension force can be added to describe the evolution of the phases.

### 1.2.2 Statistical methods

While the simplicity of the previously mentioned methods can be very attractive, the large number of discrete elements and/or resolution of the mesh required makes the methods intractable for even laboratory scale systems. For this reason, continuum methods are often preferred to describe the flows of large scale systems in which the statistical quantities of the dispersed and continuous phases are solved for instead, resulting in a large reductions in computational cost. This is due to the fact that models are used to describe the small scale interactions (momentum transfer and collisions) and do not need to be resolved, while the evolution equations describe the macro-scale motion. These transported quantities are related to the NDF of the dispersed phase inside a control volume. This includes quantities such as the volume fraction, total mass or mass density, mean velocity, and velocity variance. For most common applications, the mass density and mean quantities are tracked, however by considering more information about the local distribution, a better approximation of the NDF can be obtained.

**Method of classes** The method of classes transports a set of discretized bins approximating the dispersed phase number density function, typically using a combination of zero-order polynomials. The interaction of bins is accounted for through source terms such as aggregation, breakup, and collisions. The method of classes is often used either in the evolution of univariate distributions (Bannari et al., 2008), or for systems in which a monokinetic assumption can be made for polydisperse flows, MUSIG model (Laurent and Massot, 2001; Frank et al., 2005). The major draw...
back to the method of classes is the large amount of bins that are required to represent multivariate distributions due to the fact that the total number of bins is the product of the number of bins in each dimension of the distribution.

**Method of moments** Rather than solving for a discretized NDF, the statistical moments (number, mean, variance, etc) of the NDF are tracked and maybe used to approximate the distribution. The multivariate moments of a joint size-velocity NDF are defined as

$$M_{pijk} = \int_{R^3} \int_{R^3} \xi^p v_i^i v_j^j v_k^k f(t, x, \xi, v) dv d\xi.$$  

(1.2)

Physically, these moments can represent different quantities depending on the internal variables of the NDF, but commonly $M_{0000}$ defines the volume fraction, $M_{1000}$ the volume weighted average particle size (diameter, volume, or mass), and $\langle M_{0100}, M_{0010}, M_{0001} \rangle$ the volume weighted average velocity. The transport equation for the moments of a size-velocity distribution are obtained by multiplying Eq. (1.1) by the respective variables ($\xi$ and $v$), and integrating over the entire domain, resulting in

$$\frac{\partial M_{pijk}}{\partial t} + \nabla \cdot F_{pijk} + \int_{R^3} \int_{R^3} \xi^p v_i^i v_j^j v_k^k f(t, x, \xi, v) [A(v) + g] dv d\xi = C_{pijk}.$$  

(1.3)

The common hurdle in using the method of moments is that the moment transport equations, Eq. (1.3), are unclosed due to the fact that higher order moments are always needed in the transport of lower order moments (specifically when velocity is included). This can be solved by making assumptions about the distribution (such as the monodisperse approximation or monokinetic assumption), or through modeling of the unclosed terms. The most common example of a moment method is the Navier-Stokes Fourier equations, which describes a single fluid phase. The density is defined as the zero order moment, the mean momentum is the vector of first order moments, and the internal energy is the trace of the velocity covariance tensor of velocity. These are all used to describe the evolution of elastic particles with a shear rate proportional to the the gradient of velocity (Newtonian viscosity). One significant advantage to moment methods is that the evolved moments represent all realizations of the flow, meaning that the statistics of one simulation is representative of all flows with the same initial conditions, assuming that the flow is not turbulent. This
is unlike discrete methods in which one simulation represents one realization, and many realizations must be completed with varying initial conditions to accurately describe the average evolution of the NDF.

Two/multi-fluid model The multiphase extension of the Navier-Stokes equations is referred to as the two or multi-fluid model (Drew, 1983). In this formulation each phase is governed by a Navier-Stokes equation with additional terms to account for phases interactions including momentum and energy exchange terms. Here, both the monodisperse and monokinetic assumptions are made which leads to four transport equations that need to be solved for each phase (zero order, and the vector of first order velocity moments). This greatly reduces computational costs, but reduces the accuracy in the dilute regimes, or regions with higher Knudsen numbers. As mentioned before, polydispersity is very difficult for the two-fluid model due to the fact that only a mean diameter is used. This is often handled in one of two ways. The simplest uses an evolution equation for the mean diameter (Lo and Zhang, 2009), however this neglects any difference in the forces due to the size distribution so size segregation cannot occur at small scales. Alternatively, in place of a two-fluid model, a multi-fluid can be used, where multiple bubble "phases" are used and mass transfer between the "phases" occurs when bubbles change size. This method is typically coupled with the method of class is the MUSIG model (Laurent and Massot, 2001; Frank et al., 2005). This allows for different sizes of bubbles to have unique velocities so that segregation can occur.

Kinetic theory of granular flows The derivation of N-S-F type equations for granular gasses consisting a collection of inelastic particles was completed by Chapman et al. (1990) using the Boltzmann equation as the underlying VDF evolution equation. The only difference in the derivations for the elastic and inelastic equations is in the collisional term ($C_{pijk}$ in Eq. (1.3)). Due to this fact, the equation for the transport of granular energy in the inelastic case is very similar to that for the transport equation of thermal energy. The differences occur in the definitions of stress (viscosity), conductivity, and pressure terms. A isotropic, Maxwellian distribution is assumed for
the particle VDF, resulting in the addition of one transport equations for granular energy. This limits the range of applicability to small Knudsen number where particle collisions are dominant. However, generalizations have been made to account for anisotropy in the VDF for a monodisperse size distribution by Kong and Fox (2017), polydisperse derivations has been completed for an isotropic VDF by Gidaspow (1994); Huilin et al. (2001); Garzó et al. (2007); Kong and Fox (2019), and a derivation was completed by Chao et al. (2011) for a polydisperse, anisotropic VDF. With the exception of Kong and Fox (2017), while a variance of velocity is incorporated, the flux of the moments is only contributed to by the mean velocity.

**Quadrature-based moment methods**  The moment methods discussed prior only track the required moments and use these quantities to close the evolution equations. This requires models to be used in order to approximate the effects of the higher order moments present in the true evolution equations. In place of models to close these terms, the quadrature-based method of moments transports a set of moments, then uses this moment vector to approximate the distribution. This is done by using a summation of kernel density functions to approximate the NDF

$$n(\xi, v) \approx \sum_{\alpha} w_\alpha \delta(\xi - \xi_\alpha) \delta(v - v_\alpha) d\xi dv,$$

so that the moments are approximated

$$M_{pijk} \approx \sum_{\alpha} w_\alpha \xi_\alpha^{p} v_x^{i} v_y^{j} v_z^{k}. \quad (1.5)$$

The standard quadrature-based method of moments (for a one dimensional distribution) uses Dirac-delta distributions as the kernel density function (McGraw, 1997), however the extended quadrature based method of moments (EQMOM) uses smooth kernel density functions such as gamma, log-normal, beta, etc. (Yuan et al., 2012; Madadi-Kandjani and Passalacqua, 2015). Using this definition of the moments, we obtain a system of $2N$ or $2N + 1$ equations where $N$ is the total number of kernel density functions, or nodes. The required number of moments that must be transported are determined by the number of nodes. This then allows approximations of higher order moments to be made with the approximate distribution, as well as integration of integrals over...
the entire NDF. The exact way in which the moment sets are used to approximate the distribution will be discussed later.

The simplest application of QBMM is that applied to univariate, size distribution in which the particle Stokes number is assumed to be zero, and therefore the velocity distribution is described by the mean velocity of the surrounding fluid (Marchisio et al., 2003; Nguyen et al., 2016; Passalacqua et al., 2018). QBMM is not limited to univariate distributions though, instead any distribution can be approximated using a moment set of the distribution. Direct solutions to this problem exist, such as an iterative Newton-Raphson solution (Wright et al., 2001) or the Tensor Product (Yoon and Mcgraw, 2004), but other methods such as the conditional quadrature method of moments (CQMOM) (Yuan and Fox, 2011), or the hyperbolic conditional quadrature method of moments (CHyQMOM) (Fox et al., 2018) are typically required due to numerical limitations of poorly conditioned systems of equations or inverse of large matrices.

Due to the fact that any distribution can be reconstructed, QBMM can be applied the full range of Stokes numbers allowing for the transport of distributions with a continuous, non-trivial size-velocity distribution. This has previously been applied to both monokinetic distribution for bubbly flows (Fox et al., 2008; Vikas et al., 2011), monodisperse velocity distributions Yuan and Fox (2011); Passalacqua et al. (2011); Fox et al. (2018), and size-velocity with fixed sizes Passalacqua and Fox (2013).

1.3 Research Objectives

As mentioned previously, most derivations of multi-fluid systems are only for monodisperse particle distributions or fixed sizes. When a polydisperse size distribution is considered additional, the coupling between phases becomes non-trivial, and the distribution of size dependent forces must be included. This includes segregation of sizes due to differences in drag and lift forces that are effected by the particle sizes, and the resulting size-conditioned velocities. Additionally, polydispersity in KTGF leads to fluid properties which depend on the entire size distribution. This leads to common numerical approaches, such as the implicit treatment of the particle pressure
term, that must be modified so that a stable solution method can be obtained. For these reasons, the primary goal of this work is to develop continuum methods to accurately solve polydisperse disperse flows in a robust manner. The following topics are the primary focus:

- Couple monokinetic moment methods with a two-fluid model for the solution to polydisperse bubbly flows.

- Develop and implement a semi-implicit solution method for the particle pressure term in polydisperse, multi-fluid particulate systems.

- Develop of a size-velocity solution method to solve the generalized population balance equation.

The order in which the topics are presented are in order of increasing complexity, and the removal of assumptions placed on the underlying distributions. This is done to incrementally increase the solution accuracy and the range of applicable Stokes numbers and Knudsen numbers.

### A quadrature-based moment method for polydisperse bubbly flows

A computational algorithm for polydisperse bubbly flow is developed by combining quadrature-based moment methods (QBMM) with an existing two-fluid solver for gas–liquid flows. Care is taken to ensure that the two-fluid model equations are hyperbolic by generalizing the kinetic model for the bubble phase proposed by Biesheuvel and Gorissen (1990). The kinetic formulation for the bubble phase includes the full suite of interphase momentum exchange terms for bubbly flow, as well as ad hoc bubble–bubble interaction terms to model the transition from isolated bubbles to regions of pure air at very high bubble-phase volume fractions. A robust numerical algorithm to couple the QBMM approach with a gas–liquid two-fluid solver is proposed. The resulting algorithm is tested to show hyperbolicity, verified against the two-fluid model currently implemented into OpenFOAM, and validated against two sets of experiments on bubbly flows from the literature. In both cases the computational method shows good agreement with experimental data, and improved accuracy in comparison to other simulation techniques. Lastly the robustness of the algorithm is tested on
an unstructured mesh with a high superficial gas inlet velocity and source terms for coalescence and breakup. The resulting computational approach is implemented in the open-source CFD code OpenFOAM as part of the OpenQBMM project.

A semi-implicit solution algorithm for polydisperse granular flows A method to simulate polydisperse granular flows has been developed with the aim of allowing for general implementation, as well as ensuring solution stability. Standard methods for implicitly treating the granular flux in the volume fraction transport have been modified so that in addition to the stability added by the diffusion operator, the total mass is also conserved, this is achieved by using a semi-implicit solution procedure. Additionally flux limiters are used to ensure that the packing limit is not reached. This is done for individual granular phases, as well as the total particle volume fraction. The presented algorithm is first verified using a settling bidisperse bed to examine the difference in drag forces acting on the different particle sizes. The segregation of particles is the validated against an existing solver and to experiments using a bidisperse fluidized bed Ahmad et al. (2013). Finally the spatial distribution of particles is examined using a cyclic vertical riser with a bidisperse particle distribution and compared to the work of Chao et al. (2011 Chemical Engineering Science 66 (16), 3605-3616). All work has been completed in the OpenFOAM framework using the reactingEulerFoam solver.

A quadrature-based moment method for the evolution of the joint size-velocity number density function of a particle population A quadrature-based moment method for the approximate solution of the generalized population balance equation (GPBE) governing the evolution of the joint size-velocity number density function (NDF) of a particle population is formulated and tested. The proposed method relies on the third-order hyperbolic conditional quadrature method of moments developed by Fox et al. (2018, Journal of Computational Physics, 365, 269 - 293) for velocity distribution transport. This approach is combined with the conditional quadrature method of moments (Yuan and Fox, 2011) to incorporate the dependency of the NDF on particle size. This approach allows for an efficient, stable quadrature method that makes use
of an analytical solution to determine the size-conditioned velocity moments. The incorporation of source terms accounting for aggregation, breakup and collisions, as well as acceleration terms such as gravity and drag is discussed. The approach is then demonstrated considering zero-dimensional cases to verify the correct integration of the source terms. A set of one-dimensional cases involving droplet evaporation and coalescence are used to validate the velocity dependent source terms. A final set of two-dimensional cases of crossing jets of particles with different sizes are discussed to illustrate the predictive capability of the proposed method. All work has been implemented in the open source framework OpenQBMM.

1.4 Accomplishments

Completed tasks for the research objectives are presented in Table 1.1
Table 1.1: Description of completed tasks, results, and conclusions.

<table>
<thead>
<tr>
<th>Objectives</th>
<th>Results</th>
<th>Conclusions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop a model to accurately predict the evolution of polydisperse bubbly flows</td>
<td>1. A solution method for coupling moment transport to the two-fluid model is developed.</td>
<td>1. The method converges to a solution with increasing grid resolution showing that the model is hyperbolic</td>
</tr>
<tr>
<td></td>
<td>2. The numerical treatment of implicit force terms is handled to ensure a stable solution.</td>
<td>2. Unlike monodisperse systems, segregation of bubbles occur when a polydisperse size distribution is evolved with a low initial volume fraction.</td>
</tr>
<tr>
<td></td>
<td>3. The hyperbolicity of the equations is tested using merging 1-D bubble size distributions.</td>
<td>3. The coupled moment transport and two-fluid model produce the same results in the monodisperse limit.</td>
</tr>
<tr>
<td></td>
<td>4. The model is compared to the two-fluid model in the monodisperse limit.</td>
<td>4. Bubble plume oscillations frequencies are consistent with experimental data using a polydisperse bubble size distribution.</td>
</tr>
<tr>
<td></td>
<td>5. Validation of the oscillation frequency of a bubble column with central injection is compared to experimental data.</td>
<td>5. A stable solution is obtained with an unstructured grid and high bubble velocities.</td>
</tr>
<tr>
<td></td>
<td>6. The stability of the method is tested using an unstructured mesh with a high superficial bubble inlet velocity.</td>
<td></td>
</tr>
</tbody>
</table>
Table 1.1: Description of completed tasks, results, and conclusions.

<table>
<thead>
<tr>
<th>Objectives</th>
<th>Results</th>
<th>Conclusions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop a numerical method to increase the stability of the granular pressure term for polydisperse granular flows</td>
<td>1. The discretized form of the particle momentum equations are derived.</td>
<td>1. A settling bidisperse mixture produces the correct qualitative results of a higher volume fraction of particles at the bottom of the bed.</td>
</tr>
<tr>
<td></td>
<td>2. An algorithm to limit the total particle phase volume fraction is developed.</td>
<td>2. Time-averaged results match that of experiments for a bidisperse fluidized bed.</td>
</tr>
<tr>
<td></td>
<td>3. A semi-implicit solution method is developed to limit the individual granular phase volume fraction fluxes.</td>
<td>3. The spatial distribution of small particles in a cyclic riser match that of previous results, but the small particle distribution is over predicted at the walls due to the cyclic case setup.</td>
</tr>
<tr>
<td></td>
<td>4. A settling particle bed is simulated to validate the settling particle size distribution.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5. The size distribution of a fluidized, polydisperse bed is compared to experiments and current implementations.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6. A cyclic vertical riser is simulated to validate the average particle size segregation.</td>
<td></td>
</tr>
</tbody>
</table>
Table 1.1: Description of completed tasks, results, and conclusions.

<table>
<thead>
<tr>
<th>Objectives</th>
<th>Results</th>
<th>Conclusions</th>
</tr>
</thead>
</table>
| Develop a numerical method to solve the moment transport equation for the generalized population balance equation | 1. The moment transport equations and source terms are derived for the NDF of a size-velocity distribution  
2. A numerical algorithm is developed to evolve the size-velocity NDF due to advection as well as size and collisional sources.  
3. The solution methods is validated using 0-D source term evolution for size and collisions  
4. 1-D droplet cases are used to validate the advection, evaporation (growth), and coalescence terms | 1. 0-D results match that of univariate size distribution evolution and collisional, bidisperse velocity distributions.  
2. 1-D droplet evolution matches the results obtained using the direct quadrature based method of moments for cases not including coalescence.  
3. Coalescence results under predict the slip velocity of droplets due to insufficient distribution resolution |

1.5 Outline

The remaining work will be is organized as follows. In Chap. 2 the application of QBMM to a polydisperse, monokinetic bubble size-velocity distribution in which the evolution of the bubble size distribution is solved using both QBMM and the two fluid model to allow for a continuous bubble phase. In Chap. 3 a solution method for a system of n-discrete particle phases is presented in the multifluid framework making use of an semi-implicit formulation to ensure a stable solution. In Chap. 4 a complete formulation of the generalized population balance equation is presented to solve for the complete size-velocity distribution of a discrete phase with source terms accounting for size and velocity evolution. Finally in Chap. 5 a summary of the work is presented.
1.6 References


CHAPTER 2. A QUADRATURE-BASED MOMENT METHOD FOR POLYDISPERSE BUBBLY FLOWS

This chapter is an article titled "A quadrature-based moment method for polydisperse bubbly flows" published in *Computer Physics Communication* by J.C. Heylmun, B. Kong, A. Pasalacqua, and R.O. Fox (Heylmun et al., 2019).

2.1 Introduction

Gas–liquid bubbly flows have a wide variety of uses in the biological, chemical, nuclear energy, and petroleum industries. Bubble-column reactors, boilers, and stirred-tank reactors are several common example applications of bubbly flows where complex flow patterns can be observed. One of the most commonly used is the bubble-column reactor for its benefits of low operating cost and high rates of heat and mass transfer Díaz et al. (2008). They are regularly house to processes such as oxidation, chlorination, alkylation, polymerization, and hydrogenation Shah et al. (1982), and are used for fuel refinement, fermentation, and waste-water processing Kantarci et al. (2005). The construction of production size test reactors used for these processes can be very expensive, and there also exist problems with scale up when transitioning from smaller scale to full-size reactors. In order to alleviate these costs and uncertainties, the use of computational fluid dynamics (CFD) as a prediction method is often an attractive alternative. Validated CFD software allow flow patterns to be predicted without the need to build different scale reactors or to conduct extensive experimental campaigns.

While there are several methods to simulate gas–liquid flows, the most commonly used for large-scale, industrial applications is the Euler–Euler (EE) two-fluid approach Drew (1983). The EE methodology uses two continuous phases rather than a continuous liquid phase and a discrete dispersed phase, as in the case of the Euler – Lagrange method. This allows for more computational
tractable simulations when large-scale geometries are considered. The simplest form of the two-fluid model solves for the phase mass, the mean phase velocities, and a single shared pressure. The gas-phase mass and mean momentum are the lower-order moments of the bubble joint size–velocity distribution. Because the two-fluid model only tracks the first-order moments, higher-order statistics, such as size and velocity variance, are neglected. Therefore, only a single bubble diameter is considered (Sauter mean). While the velocity variance for a given bubble size is not important due to the low Stokes number of the bubbles, there exists a distribution of velocities due to the balancing of drag and buoyancy forces and their strong dependence on the bubble diameter. These phenomena cannot be captured by two-fluid models coupled with a population balance under the assumption that all the bubbles in a computational cell move with the same mean velocity Sanyal et al. (2005); Petitti et al. (2010). In addition, the basic EE formulation also suffers from not being hyperbolic and, therefore, cannot reach a converged solution with grid refinement Stewart and Wendroff (1984); Ndjinga (2007); Panicker et al. (2018). A strategy to enforce hyperbolicity of the multi-fluid model is discussed in Kumbaro and Ndjinga (2011).

In order to simulate a wide distribution of bubble sizes, and, consequently, of velocities, a multi-fluid model can be used, where each bubble size is treated as a unique gas phase, allowing each bubble size to have a unique velocity. However, when bubble breakup and coalescence are significant, models for mass transfer between bubble sizes must also be included. The algorithms to advect the phase volume fraction while ensuring its boundedness are often more complicated and expensive than those for two-phase flows. While not able to handle the full range of bubbly flows, previous authors have used a weak coupling method to simulate polydisperse bubbly flows. This can be accomplished by coupling a dispersed gas phase and a continuous liquid phase through drag, and using a quadrature-based method of moments (QBMM) to close the moment transport equations Marchisio and Fox (2013); Yuan et al. (2014); Buffo et al. (2013); Vikas et al. (2011). However, existing QBMM methodologies Yuan et al. (2014) do not allow for regions of pure gas, as the pressure would become undefined, being it define from the continuity equation of the fluid phase only. A somewhat simpler moment method developed by Lo and Zhang (2009) tracks only the zeroth
through third order moments in order to calculate $d_{32}$, or the volume weighed diameter. From this only a mean diameter is obtained and used in the calculations of source terms. This also assumes that velocity bubble distribution can be described using only the mean velocity. Another method to simulate polydisperse gas-liquid systems is the class method, in which the bubble size distribution is separated into bins, and the bubbles in each bin interact Selma et al. (2010). This has many of the same benefits of QBMM, however, in general it is more computationally expensive because a large number of bins is required to accurately describe the bubble size-velocity distribution, and each bin must be transported in physical space with its own velocity. The most commonly used class method is the MUSIG scheme (Frank et al., 2005) in which a multi-fluid model is used to represent the bubble phases, where each phase represents a bin of the approximate distribution. This approach is a commonly used model in the nuclear industry to simulate boiling Ho et al. (2008); Yeoh and Tu (2006). This model uses exchange terms in the continuity, momentum and energy equations to account for the breakup and coalescence of bubbles, introducing additional cost and difficulty in solving the model equations. Alternative approaches are therefore needed that can accurately and robustly simulate polydisperse gas-liquid flows while maintaining a moderate computational cost.

In this work, a numerical algorithm for the simulation of polydisperse bubbly flows is developed starting from a kinetic equation describing the evolution of the joint size-velocity number density function (NDF) of the bubbles. The size and velocity moments of the kinetic equation are transported, and closure of the moment transport equations is achieved by means of QBMM. In order to overcome the numerical difficulties encountered in previously developed QBMM for gas-liquid systems Yuan et al. (2014), which presented limitations in their capability of dealing with extreme cases where areas of pure gas are present, the liquid and gas phases are coupled through the two-fluid model, where the gas phase is treated as a continuum and is coupled to the liquid phase through interfacial forces (such as buoyancy, drag, virtual mass, etc.) and the pressure equation. The mean quantities, or first-order moments, are solved using a modified version of the numerical procedure traditionally used in the two-fluid model in OpenFOAM Weller (2005, 2006); OpenCFD Ltd. (2018), which has proven robust in managing absence of a phase and in maintaining
the boundedness of the volume fraction field. The remaining additional moments are computed using the moment transport equations. The interface coupling terms are also modified to include contributions arising from the polydisperse nature of the flow and by its description with QBMM. In addition, the hyperbolicity of the model is enforced by using a dispersion term Panicker et al. (2018), proportional to the gradient of the gas volume fraction.

Here, the solution of the system of partial differential equations for the moments of the NDF is obtained by decomposing the vector of transported moments into two components: one representing the mean and the other the deviation with respect to the mean. An iterative algorithm for the solution of two-fluid model equations Spalding (1980, 1983) is used to solve for the volume fraction and the mean velocity (first-order moments) of the bubble phase, in order to ensure boundedness of the numerical solution and to enable the robust calculation of the fluid pressure in extreme situations when the liquid phase is locally absent. QBMM, combined with realizable convection schemes Perthame (1992); Vikas et al. (2011), is used to transport higher-order moments of the bubble size distribution. Operator splitting is employed to separate spatial advection from other physical processes such as bubble coalescence and breakage. Results obtained with the proposed computational algorithm are then verified against base Euler–Euler two-phase solver in the monodisperse limit, and then validated against experiments Pfleger et al. (1999); Díaz et al. (2008) with a distribution of bubble sizes. A challenging example is provided showing, the ability of the proposed algorithm to account for bubble coalescence and breakage in a system with non-trivial geometry, spatially discretized with an unstructured mesh.

The remainder of the paper is organized as follows. In Sec. 2.1.1, details concerning the computational model for bubbly flows are provided with emphasis on the kinetic model used to describe polydisperse gas-liquid flows. In Sec. 2.1.2 the interphase force terms needed for bubbly flows are reviewed, focusing on their extension to polydisperse cases. Sec. 2.1.3 is devoted to describing how QBMM is employed to treat the polydisperse bubbly flow equations, expressed in terms of the moments of the kinetic model introduced in Sec. 2.1.1. The numerical algorithm for polydisperse bubbly flow is then presented in Sec. 2.1.4. Focus is put on how the terms arising from
polydispersity are treated in the context of the two-fluid solver for monodisperse flows available in OpenFOAM (e.g., twoPhaseEulerFoam), which is based on the IPSA algorithm of Spalding (1980, 1983). Example applications of the proposed algorithm are presented in Sec. 2.1.5, and conclusions are drawn in Sec. 2.1.6.

2.1.1 Computational Model for Bubbly Flow

In this section a set of governing equations for bubbly flows, based on a generalization of the kinetic model derived by Biesheuvel and Gorissen Biesheuvel and Gorissen (1990), referred to hereinafter as the Biesheuvel and Gorissen model, is proposed. This extension is necessary because the original Biesheuvel and Gorissen model was derived for a one-dimensional flow involving monodisperse bubbles with drag, added-mass and buoyancy forces. The generalization proposed in the present work reduces to the Biesheuvel and Gorissen model in the appropriate one-dimensional limit. A hydrodynamic model for the liquid phase and a kinetic model for the bubble phase that retain the important physical and mathematical properties of the Biesheuvel and Gorissen model are then proposed.

2.1.1.1 Bubble-phase description in Biesheuvel and Gorissen model

In the absence of mass transfer between phases, the spatial-temporal evolution of the volume fraction of the bubble phase in monodisperse bubbly flows can be described by a continuity equation

\[ \frac{\partial \rho_b \varepsilon_b}{\partial t} + \nabla \cdot (\rho_b \varepsilon_b \mathbf{U}_b) = 0, \quad (2.1) \]

which is coupled to the liquid-phase governing equations through the constraint

\[ \varepsilon_l + \varepsilon_b = 1 \quad (2.2) \]

where \( \varepsilon_l \) and \( \varepsilon_b \) are the liquid-phase and bubble-phase volume fractions, respectively. The gas density \( \rho_b \) is assumed to be constant, and can be divided out of Eq. (2.1). \( \mathbf{U}_b \) is the bubble-phase velocity vector. In the one-dimensional limit, Eq. (2.1) reduces to equation [34] in Biesheuvel and Gorissen Biesheuvel and Gorissen (1990).
The momentum equation for the bubble phase in the Biesheuvel and Gorissen model is
\[
\frac{\partial \rho_b \varepsilon_b U_b}{\partial t} + \nabla \cdot (\rho_b \varepsilon_b U_b \otimes U_b) = \nabla \cdot \tau_b - \nabla p_b + \rho_b \varepsilon_b g - M_{lb},
\]
(2.3)
where \( p_b \) is the bubble-phase pressure generated by hydrodynamic interaction in the liquid phase. \( M_{lb} \) is the momentum-exchange term between the liquid and bubble phases, which includes the liquid-pressure force on the bubbles, equal to \( \varepsilon_b \nabla p_l \), and \( g \) is the gravitational acceleration vector. The bubble-pressure model proposed by Biesheuvel and Gorissen Biesheuvel and Gorissen (1990) has the form
\[
p_b = C_{bp} (\rho_b + \rho_l C_{vm}) \varepsilon_b |U_l - U_b|^2 H(\varepsilon_b),
\]
(2.4)
where \( \rho_l \) is the liquid density. The constant \( C_{bp} \) is of order one, and \( U_l \) is the liquid velocity. The function
\[
H(\varepsilon_b) = \varepsilon_b \varepsilon_l,
\]
(2.5)
was introduced by Batchelor Batchelor (1988) and retained by Biesheuvel and Gorissen Biesheuvel and Gorissen (1990) to model the volume-fraction dependence of the hydrodynamic interactions between bubbles. As pointed out by Batchelor Batchelor (1988), the magnitude of the velocity fluctuations in the liquid phase due to the presence of the bubbles (i.e. pseudo-turbulence Magnaudet and Eames (2000); Prakash et al. (2016)), modeled as \( C_{bp} |U_l - U_b|^2 H(\varepsilon_b) \), can be validated using experiments Prakash et al. (2016) or microscale DNS Tenneti and Subramaniam (2014).

The added-mass coefficient \( C_{vm} \) is modeled by Biesheuvel and Spoelstra (1989); Zuber (1964)
\[
C_{vm} = \frac{1 + 2\varepsilon_b}{2\varepsilon_l}.
\]
(2.6)
As the bubble-phase volume fraction approaches unity, the pressure in Eq. (2.4) is dominated by \( C_{vm} H \sim 1 \), and thus the bubble-phase pressure will not be null.

In Eq. (2.3), the bubble-phase deviatoric stress tensor \( \tau_b \) is modeled as
\[
\tau_b = (\rho_b + \rho_l C_{vm}) \varepsilon_b \nu_b \left[ \nabla U_b + (\nabla U_b)^T - \frac{2}{3} (\nabla \cdot U_b) I \right],
\]
(2.7)
where \( I \) is the unit tensor and \( \nu_b \) is the bubble-phase kinematic viscosity Biesheuvel and Gorissen (1990)
\[
\nu_b = C_b d_b |U_l - U_b|\sqrt{H(\varepsilon_b)}, \quad C_b = O(1),
\]
(2.8)
where $d_b$ is the bubble diameter. As the bubble-phase volume fraction approaches unity, the viscosity in Eq. (2.7) is dominated by $C_{vm}\sqrt{H} \sim 1/\sqrt{\varepsilon}$, and thus the bubble-phase viscosity will become very large.

The interfacial forces acting on the bubble phase from the liquid phase include drag, virtual mass, buoyancy and lift. In the Biesheuvel and Gorissen model, the lift force is zero and $C_{vm}$ is used as the virtual-mass coefficient. The buoyancy force arises in the Biesheuvel and Gorissen model due to static pressure: $\nabla p_l = \rho_l g$, where $g$ is the gravitational acceleration vector. Compared to the standard drag force model, the Biesheuvel and Gorissen model includes a dispersion term

$$F^D = \frac{\rho_b}{\tau_D} \left[ \varepsilon_b (U_l - U_b) - \delta_{\text{dis}} \nabla \varepsilon_b \right], \quad (2.9)$$

where $\tau_D$ is the drag time scale and the dispersion coefficient is modeled by Batchelor (1988)

$$\delta_{\text{dis}} = C_{\text{dis}} d_b |U_l - U_b| \sqrt{H(\varepsilon_b)}, \quad C_{\text{dis}} = O(1). \quad (2.10)$$

Eq. (2.9) has the same form as the model used by Davidson (1990) and Drew and Lahey (1980). As with the other terms involving $H$, the dispersion term arises due to hydrodynamic interactions between bubbles through the liquid phase.

In summary, the novel features of the Biesheuvel and Gorissen model, in comparison to the standard two-fluid model, are the three terms representing hydrodynamic interactions: $p_b$, $\nu_{b,\text{eff}}$ and $\delta_{\text{dis}}$. Analysis of the one-dimensional two-fluid model in the inviscid limit (Panicker et al., 2018) reveals that $\delta_{\text{dis}}$ is crucial to guarantee the correct mathematical properties of the set of partial differential equations. In the context of polydisperse bubbly flows, we must therefore include the hydrodynamic interaction terms in order to obtain the correct behavior in the monodisperse limit. However, because the properties of the two-fluid model in the inviscid limit depend on the form of both the bubble and the liquid phase momentum balances, it is possible to treat the bubble pressure as an interfacial force Ndjinga (2007) and thus to include it in the definition of $M_{lb}$. Likewise, the effective kinematic viscosity can be added to the liquid phase in a manner such that the overall effective viscosity of the mixture is nearly unchanged. With these modifications, the momentum
equation for the bubble phase in the dilute, monodisperse limit becomes
\[
\frac{\partial \rho_b \varepsilon_b U_b}{\partial t} + \nabla \cdot (\rho_b \varepsilon_b U_b \otimes U_b) = \rho_b \varepsilon_b \mathbf{g} - M_{lb}
\]
(2.11)
where \( M_{lb} \) now includes the dispersion and bubble-pressure terms written as forces acting on individual bubbles. The exact definition of \( M_{lb} \) will be given below when we introduce the kinetic description of the bubble phase.

2.1.1.2 Liquid phase

The continuity equation for the liquid phase is
\[
\frac{\partial \rho_l \varepsilon_l}{\partial t} + \nabla \cdot (\rho_l \varepsilon_l U_l) = 0,
\]
(2.12)
where the liquid density is assumed constant. The momentum equation for the liquid phase is
\[
\frac{\partial \rho_l \varepsilon_l U_l}{\partial t} + \nabla \cdot (\rho_l \varepsilon_l U_l \otimes U_l) = \nabla \cdot \tau_l - \nabla (p_l + p_b) + \rho_l \varepsilon_l \mathbf{g} + M_{lb}.
\]
(2.13)
The liquid-phase pressure includes \( p_b \), representing the liquid-velocity fluctuations due to hydrodynamic interactions. The deviatoric stress tensor \( \tau_l \) is modeled as
\[
\tau_l = \rho_l \varepsilon_l \nu_{l,\text{eff}} \left[ \nabla U_l + (\nabla U_l)^T - \frac{2}{3} (\nabla \cdot U_l) \mathbf{I} \right],
\]
(2.14)
where \( \nu_{l,\text{eff}} \) is defined as the sum of the liquid kinematic viscosity and a contribution due to hydrodynamic interactions:
\[
\nu_{l,\text{eff}} = \nu_l + \frac{\varepsilon_b}{\varepsilon_l} \left( \frac{\rho_b}{\rho_l} + C_{vm} \right) \nu_b.
\]
(2.15)
As noted earlier, due to the definition of \( C_{vm} \), \( \nu_{l,\text{eff}} \) becomes very large when the bubble-phase volume fraction approaches unity. The volumetric velocity \( \mathbf{U}_{\text{vol}} = \varepsilon_b \mathbf{U}_b + \varepsilon_l \mathbf{U}_l \), is solenoidal \( (\nabla \cdot \mathbf{U}_{\text{vol}} = 0) \), thereby defining the algebraic constraint needed to determine \( p_l \).

In the following, we will assume that the liquid-phase continuity and momentum equations are given by Eqs. (2.12) and (2.13), respectively. These equations are coupled to the kinetic equation for the bubble phase introduced below, through \( \varepsilon_b, \mathbf{U}_b \) and \( M_{lb} \). All of the parameters depending on \( \varepsilon_b \) and \( \mathbf{U}_b \) remain the same as defined above, unless indicated otherwise.
2.1.1.3 Polydisperse bubble phase

The bubble-phase governing equation is represented by a kinetic equation Vikas et al. (2011); Marchisio and Fox (2013); Yuan et al. (2014) for the joint mass–velocity bubble NDF $f(t, x, \xi, v)$, defined so that $\int d\xi\,dv$ is the average number of bubbles with mass between $\xi$ and $\xi + d\xi$, velocity between $v$ and $v + dv$, and position between $x$ and $x + dx$ at time $t$. The general form of the kinetic equation describing the evolution of $f(t, x, \xi, v)$ is

$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{\partial}{\partial v} \left[(A + g)f - D \cdot \frac{\partial \ln n}{\partial x} f\right] = C(\xi, v)$$ \hspace{1cm} (2.16)

where $n(\xi) = \int f \, dv$ is the marginal NDF for bubble size. The term $A$ represents acceleration due to the forces acting on an individual bubble, as will be described in detail below. The term involving the second-order tensor $D(\xi, v)$ represents acceleration due to the dispersion forces, which depends on spatial gradients of the bubble-phase NDF. The term $C$ represents binary interactions of bubbles. When breakup and coalescence are considered, this term will also account for the change in bubble sizes due to interaction with other bubble sizes. In their absence, $C$ accounts for changes in the bubble momentum for bubbles with different sizes and velocities, and for spatial fluxes due to bubble–bubble interactions mediated by the fluid phase. For gas–particle flows, $C$ is primarily due to collisions and analytical expressions can be derived Marchisio and Fox (2013). For bubbly flows, phenomenological models are proposed below.

With QBMM the solution of the kinetic equation is approximated by tracking the spatio-temporal evolution of moments of the joint NDF instead of the joint NDF itself Marchisio and Fox (2013). The transport equations for these moments can be written as

$$\frac{\partial m_{p,i,j,k}}{\partial t} + \frac{\partial m_{p,i+1,j,k}}{\partial x} + \frac{\partial m_{p,i,j+1,k}}{\partial y} + \frac{\partial m_{p,i,j,k+1}}{\partial z} = F_{p,i,j,k} - iD_{p,i,j,k}^{x} - jD_{p,i,j,k}^{y} - kD_{p,i,j,k}^{z} + C_{p,i,j,k},$$ \hspace{1cm} (2.17)

where the right-hand side is defined by an integral over the mass–velocity phase space, where, for brevity, the dependence on $t$ and $x$ is suppressed. The terms on the right-hand side of Eq. (2.17)
are defined considering \( \mathbf{v} \in \mathbb{R}^3 \) and \( \xi \in \mathbb{R} \):

\[
F_{p,i,j,k} = \int \xi^p v_x^i v_y^j v_z^k \left[ iv_x^{-1}(g_x + A_x) + jv_y^{-1}(g_y + A_y) + kv_z^{-1}(g_z + A_z) \right] f \, d\xi \, dv,
\]

(2.18)

\[
D_{p,i,j,k}^x = \int \xi^p v_x^{i-1} v_y^j v_z^k D_x(\xi, \mathbf{v}) \frac{\partial \ln n}{\partial x} f \, d\xi \, dv,
\]

(2.19)

\[
D_{p,i,j,k}^y = \int \xi^p v_x^{i-1} v_y^j v_z^k D_y(\xi, \mathbf{v}) \frac{\partial \ln n}{\partial y} f \, d\xi \, dv,
\]

(2.20)

\[
D_{p,i,j,k}^z = \int \xi^p v_x^i v_y^{j-1} v_z^k D_z(\xi, \mathbf{v}) \frac{\partial \ln n}{\partial z} f \, d\xi \, dv,
\]

(2.21)

\[
C_{p,i,j,k} = \int \xi^p v_x^i v_y^j v_z^k C d\xi d\mathbf{v} = C_{p,i,j,k} - \nabla_x \cdot \mathbf{G}_{p,i,j,k},
\]

(2.22)

and the moments by

\[
m_{p,i,j,k} = \int \xi^p v_x^i v_y^j v_z^k f(\xi, \mathbf{v}) \, d\xi \, dv.
\]

(2.23)

The dispersion coefficients on the right-hand side of Eq. (2.17) are defined by the components of \( \mathbf{D} \). For example, \( D_x = D_{xx} + D_{yx} + D_{zx} \). In the models developed below, the dispersion tensor is assumed to be isotropic \( \mathbf{D} = D_{\text{dis}}(\xi, \mathbf{v}) \mathbf{I} \), but in general this is not necessarily the case. The source term describing the interaction between bubbles \( C_{p,i,j,k} \) and spatial flux \( \mathbf{G}_{p,i,j,k} \) require closures. In the absence of coalescence and breakage, \( C_{p,0,0,0} = 0 \) and \( \mathbf{G}_{p,0,0,0} = \mathbf{0} \) for all \( p \).

Note that the higher-order moments in the spatial transport terms on the left-hand side of Eq. (2.17) are not closed, and thus QBMM are introduced to attain closure. In QBMM, one possible reconstruction of \( f(\xi, \mathbf{v}) \) is obtained by inverting a truncated set of its moments Fox (2014), and the latter is defined by choosing a small set of integer values for the indices \((p, i, j, k)\). The NDF reconstruction is then used to evaluate the unclosed terms in the moment transport equations Marchisio and Fox (2013). In general, it will be nontrivial to reconstruct the joint mass–velocity NDF from its moments due to its high phase-space dimensionality (i.e., four dimensions), so simplifications under reasonable physical assumptions are necessary for us to continue.
The lower-order moments defined by Eq. (2.23) have particular physical significance Marchisio and Fox (2013). For example, the first-order moment
\[ m_{1,0,0,0} = \rho_b \epsilon_b. \]
Thus, the bubble-phase continuity equation is found from Eq. (2.17) by setting \((p,i,j,k) = (1,0,0,0)\). Likewise, the moments
\[ m_{1,1,0,0} = \rho_b \epsilon_b U_{bx}, \quad m_{1,0,1,0} = \rho_b \epsilon_b U_{by}, \quad m_{1,0,0,1} = \rho_b \epsilon_b U_{bz} \]
define the mean bubble velocity \( U_b \), and their transport equations yield the bubble-phase momentum equation. For this reason, the coupling terms \( \epsilon_b \) and \( M_{lb} \) in Eq. (2.12) and Eq. (2.13) are found by integrating over mass–velocity phase space and, hence, will be known if \( f(\xi, v) \) is known Vikas et al. (2011).

2.1.1.4 Monokinetic approximation

For bubbly flow, the fluid drag falls into the low-Stokes-number regime, and thus the crossing of bubble trajectories is negligible Marchisio and Fox (2013); Fox (2014). This means that at a specific location \( x \) only one velocity exists for a given bubble mass \( \xi \), i.e., the bubble phase is monokinetic. Therefore, the joint mass–velocity NDF can be approximated as
\[ f(\xi, v) = n(\xi) \delta(v - U(\xi)), \tag{2.24} \]
where \( n(t, x, \xi) \) is the NDF based on the bubble mass, \( \delta(v) \) is the Dirac delta distribution, and \( U(t, x, \xi) \) is the bubble velocity conditioned on mass. With QBMM, \( n(\xi) \) is reconstructed from the \( 2N \) moments \( M_p = m_{p,0,0,0} \) for \( p \in \{0,1,\ldots,2N-1\} \). The functional form for \( U(\xi) \) is found from the moments \( U_p = (m_{p,1,0,0}, m_{p,0,1,0}, m_{p,0,0,1}) \) for \( p \in \{0,1,\ldots,N-1\} \). Thus, Eq. (2.17) must be solved for these \( 5N \) moments. For the special case of monodisperse bubbly flow, only the four moments with \( p = 1 \) are used.

Using the approximation in Eq. (2.24), we can formally rewrite the kinetic equation in Eq. (2.16) in a more familiar form. First, integrating Eq. (2.24) with respect to the velocity \( v \) yields
\[ \frac{\partial n}{\partial t} + \nabla \cdot [nU(\xi)] = C(\xi), \tag{2.25} \]
i.e., a population balance equation for \( n \). Then, multiplying Eq. (2.24) by \( v \) and integrating with respect to the velocity yields
\[ \frac{\partial nU}{\partial t} + \nabla \cdot [nU \otimes U + G(\xi)] = ng + A(\xi, U)n - D_{dis}(\xi, U)\nabla n + C(\xi), \tag{2.26} \]
i.e., a momentum balance for $U$. Here $A(\xi, U)$ is the size-dependent acceleration terms evaluated at the mass-dependent velocity. The dispersion term in Eq. (2.26) was placed on the right-hand side as it represents a force shared with the fluid phase (see Eq. (2.9) where $D_{\text{dis}} = \delta_{\text{dis}}/\tau_D$), and not a spatial flux. The bubble–bubble interaction term in Eq. (2.26) is written as a source term and a spatial flux. The source term can be modeled by

$$C(\xi) = \frac{\varepsilon_b g_0(\varepsilon_b)}{\tau_c} [U_b - U(\xi)] n(\xi) + \int_0^{\infty} \xi^p U(\xi) C d\xi,$$  \hspace{1cm} (2.27)$$

where $g_0$ is one for small $\varepsilon_b$ and grows rapidly as $\varepsilon_b$ approaches close-packed conditions so that the bubble velocity becomes independent of size. The spatial flux can be modeled as

$$G(\xi) = \frac{1}{\rho_b \varepsilon_b} (p_c I - \tau_c) n(\xi),$$  \hspace{1cm} (2.28)$$

where the pressure $p_c(\varepsilon_b)$ and the deviatoric stress tensor $\tau_c(\varepsilon_b)$ are nonzero only when $\varepsilon_b$ is greater than 0.63 (i.e., the dense bubbly phase is modeled as a foam with its own equation of state and viscous stress tensor Bonn et al. (2017)). In the monodisperse limit, Eq. (2.26) reduces to Eq. (2.11) when $\varepsilon_b < 0.63$.

The system of Eq. (2.25) and Eq. (2.26) has the form of hyperbolic conservation laws. As we shall see later, the force terms in $A$ do not involve spatial derivatives of $U$, and thus the solution $U$ to Eq. (2.26) need not be a continuous function of $x$. Moreover, it is important to note that both $n$ and $U$ are continuous functions of $\xi$, and, thus, that Eq. (2.25) and Eq. (2.26) represent an infinite set of bubble-phase continuity and momentum equations, one set for each real value of $\xi$.

The transport equation for the moment $M_p = \int \xi^p n d\xi$ is found from Eq. (2.25), while that for the vector $U_p = \int \xi^p U(\xi) n d\xi$ is found from Eq. (2.26). These equations are

$$\frac{\partial M_p}{\partial t} + \nabla \cdot U_p = \int_0^{\infty} \xi^p C d\xi$$  \hspace{1cm} (2.29)$$
and
\[
\frac{\partial \xi U_b}{\partial t} + \nabla \cdot \left[ P_p + \frac{M_p}{\rho_{b} \varepsilon_b} (p_c I - \tau_c) \right] = M_p g + \int_0^\infty \xi^p (A - D_{dis} \nabla \ln n) n \, d\xi + \frac{\xi_b g_0}{\tau_c} (M_p U_b - U_p) + \int_0^\infty \xi^p U(\xi) C \, d\xi. \quad (2.30)
\]

The second-order tensor \( P_p \) is defined in terms of \( U(\xi) \) by
\[
P_p = \int_0^\infty \xi^p U(\xi) \otimes U(\xi) n \, d\xi. \quad (2.31)
\]

For convenience, we define \( V(\xi) = U(\xi) - U_b \). Note that the second term from the right in Eq. (2.30) can be rewritten in terms of \( V_p = \int_0^\infty \xi^p V(\xi) n \, d\xi \),
\[
V_p = \int_0^\infty \xi^p V(\xi) n \, d\xi, \quad (2.32)
\]
and has the effect of forcing \( V_p \) to zero when \( g_0 \) is large (i.e., dense bubbly flow). We can then decompose the convective flux as \( P_p = P_{p,b} + P_{p,v} \) where \( P_{p,b} = U_b \otimes U_b \) and
\[
P_{p,v} = \int_0^\infty \xi^p V(\xi) \otimes U(\xi) n \, d\xi. \quad (2.33)
\]

Physically, \( \nabla \cdot P_{p,b} \) is the convective flux of \( U_b \) by the mass-average bubble velocity, and \( \nabla \cdot P_{p,v} \) is the convective flux of \( U_b \) by \( V(\xi) \). In dense bubbly flows, \( P_{p,v} \) will be negligible. These fluxes, and the next-to-last term in Eq. (2.30), depend on the reconstruction of the NDF. We will return to the question of how this is done with QBMM in Sec. 2.1.3, after defining the force terms for bubbly flow, which are needed to define \( A \) and \( D_{dis} \) in Eq. (2.30). The last term, \( C \), represents the change in the bubble size due to bubble coalescence.

### 2.1.2 Interphase Forces and Exchange Terms in Bubbly Flow

The force balance on an individual bubble with a fixed mass \( \xi \) and velocity \( U(t) \) can be written as
\[
\xi \frac{dU}{dt} = F^G + F^B + F^D + F^{VM} + F^L + F^W + F^{BP}, \quad (2.34)
\]
and the bubble position is found from the solution of \( \frac{dx}{dt} = U \). Each of the forces appearing on the right-hand side of Eq. (2.34) will be described separately below. For a monodisperse bubbly flow, \( \xi = \xi_b = \rho_b \pi d_b^3/6 \) where \( d_b \) is the bubble diameter, and \( U(\xi_b) = U_b \). In a polydisperse bubbly flow, the bubble volume is equal to \( \xi/\rho_b \), therefore the interfacial forces will be proportional to \( \xi/\rho_b \) whereas body forces will be proportional to \( \xi \). Finally, the bubble–bubble interaction terms will be important when \( \varepsilon_b \) approaches 0.63 (i.e., close-packed conditions), and these terms are neglected in Eq. (2.34), but appear in Eq. (2.30).

In the following, to simplify the notation we do not show the explicit dependence of model quantities on \( \xi \). However, the reader should keep in mind that the bubble diameter \( d_b \) is a function of \( \xi \), and thus any parameter involving \( d_b \) is an implicit function of \( \xi \) (e.g., \( K_{\text{drag}}, \text{Re}_b, \text{Eo}, \text{etc.} \)). Generally speaking, the constants in the force models can depend on \( \xi \).

### 2.1.2.1 Gravitational force \( F_{mG} \)

The gravitational force is a body force that is calculated as

\[
F^G = \xi g. \tag{2.35}
\]

### 2.1.2.2 Buoyancy force \( F_{mB} \)

The buoyancy force is an interfacial force that is modeled as

\[
F^B = -\frac{\xi}{\rho_b} (\nabla p_l - \nabla \cdot \tau^*_l), \tag{2.36}
\]

where \( \tau^*_l \) is the part of the liquid-phase deviatoric stress tensor depending on the fluid viscosity \( \nu_l \).

### 2.1.2.3 Drag force \( F_{mD} \)

The drag force is an interfacial force that is modeled as

\[
F^D = K_{\text{drag}} \left[ \frac{\xi}{\rho_b} (U_l - U) - \frac{\delta_{\text{dis}}}{\varepsilon_1} \nabla \ln n(\xi) \right], \tag{2.37}
\]

where \( \delta_{\text{dis}} \) is the dispersion coefficient arising from hydrodynamic interactions. The latter are represented by \( \nabla \ln n(\xi) \), which depends on \( \xi \), and is included in Eq. (2.30) as the term involving
\[ D_{\text{dis}} = K_{\text{drag}} \delta_{\text{dis}}/\varepsilon_1. \] Based on the Biesheuvel and Gorissen model in Eq. (2.9), the dispersion coefficient is

\[ \delta_{\text{dis}} = C_{\text{dis}} d_b |U_1 - U| \sqrt{H(\varepsilon_b)}, \tag{2.38} \]

with \( C_{\text{dis}} \approx 1. \) The drag coefficient is modeled by

\[ K_{\text{drag}} = \frac{3C_D \rho_l |U_1 - U|}{4d_b}. \tag{2.39} \]

The bubble diameter \( d_b \) is found from the bubble mass \( \xi \), assuming that bubbles are spherical.

The drag coefficient \( C_D \) is computed from Tomiyama (1998)

\[ C_D = \max \left\{ \min \left[ \frac{A}{\text{Re}_b} \left( 1 + 0.15 \text{Re}_b^{0.687} \right), 3A \right] \frac{8 \ E_o}{3 \ E_o + 4} \right\}, \tag{2.40} \]

where \( A = 16 \) for pure water or \( A = 24 \) for contaminated water. The slip Reynolds number for the gas phase is defined as

\[ \text{Re}_b = \frac{\rho_l d_b |U_1 - U|}{\mu_l}. \tag{2.41} \]

The Eötvös number is defined as Tomiyama (1998)

\[ E_o = \frac{(\rho_l - \rho_b)gd_b^2}{\sigma_b}, \tag{2.42} \]

where \( g \) is the magnitude of the gravitational acceleration and \( \sigma_b \) is surface tension, accounts for the effect of non-spherical on the drag force. In bubbly flows, \( \text{Re}_b \) is often quite large Magnaudet and Eames (2000), while the Stokes number \( \text{St} = \rho_b \text{Re}_b / \rho_l \) is very small due to the density ratio.

### 2.1.2.4 Virtual-mass force \( F_{\text{vm}} \)

The virtual-mass force is modeled as Biesheuvel and Spoelstra (1989)

\[ F_{\text{vm}} = \frac{\xi}{\rho_b} \frac{d\rho_l C_{\text{vm}} (U_1 - U)}{dt} = \frac{\xi}{\rho_b} \rho_l C_{\text{vm}} \left( \frac{dU_1}{dt} - \frac{dU}{dt} \right), \tag{2.43} \]

where \( C_{\text{vm}} \) is defined by Eq. (2.6). The time derivative of average quantities is taken along the mean path of the bubbly phase:

\[ \frac{dU_1}{dt} = \frac{\partial U_1}{\partial t} + U_b \cdot \nabla U_1. \tag{2.44} \]
Note that the virtual mass force modifies the bubble mass on the left-hand side of Eq. (2.34) by the virtual mass factor
\[ \gamma_{vm} = 1 + C_{vm} \rho_l / \rho_b. \] (2.45)
For gas–liquid flows, we can observe that \( \gamma_{vm} \approx C_{vm} \rho_l / \rho_b \gg 1 \) and thus that the added-mass effect will be important in unsteady flows.

### 2.1.2.5 Lift force \( F_{mL} \)

The lift force is modeled as Auton (1987)
\[ F_L = \frac{\xi}{\rho_b} C_L \rho_l (U_1 - U) \times (\nabla \times U_1), \] (2.46)
where the lift force coefficient is found from Tomiyama et al. (2002)
\[ C_L = \begin{cases} 
\min \{0.288 \tanh(0.121 \text{Re}_b), f(\text{Eo}_d)\} & \text{for } \text{Eo}_d < 4 \\
 f(\text{Eo}_d) & \text{for } 4 \leq \text{Eo}_d \leq 10.7 \\
 -0.27 & \text{for } \text{Eo}_d > 10.7 
\end{cases} \] (2.47)
with
\[ f(\text{Eo}_d) = 0.00105 \text{Eo}_d^3 - 0.0159 \text{Eo}_d^2 - 0.0204 \text{Eo}_d + 0.474. \]
Here \( \text{Eo}_d \) is defined as in Eq. (2.42), where \( d_b \) is replaced by the maximum horizontal diameter of the bubble \( d_h \), obtained from Wellek et al. (1966)
\[ d_h = d_b (1 + 0.163 \text{Eo}_d^{0.757})^{1/3}. \] (2.48)

### 2.1.2.6 Wall force \( F_{mW} \)

The wall force, due to lubrication forces in the liquid when a bubble approaches a solid surface Antal et al. (1991), is modeled as
\[ F_W = -\frac{\xi}{\rho_b} \nabla p_w. \] (2.49)
In this expression, the wall pressure is modeled by
\[ p_w = C_w \rho_l |U_1 - U|^2 \frac{d_b}{|x - x_w|}, \] (2.50)
where $|\mathbf{x} - \mathbf{x}_w|$ is the distance to the closest wall and $C_w = 0.0217$ Hosokawa et al. (2002). Alternatively, Antal et al. (1991) derived a wall-force model using inviscid flow theory for a single spherical bubble with diameter $d_b$. From this theory, the wall pressure can be written as

$$p_w = \rho_l |\mathbf{U}_1 - \mathbf{U}|^2 \frac{d_b}{|\mathbf{x} - \mathbf{x}_w|} \left( a_0 - a_1 \frac{d_b}{|\mathbf{x} - \mathbf{x}_w|} \right.$$

$$+ a_2 \frac{d_b^2}{|\mathbf{x} - \mathbf{x}_w|^2} + a_3 \frac{d_b^3}{|\mathbf{x} - \mathbf{x}_w|^3} \left. \right) . \quad (2.51)$$

Antal et al. (1991) applied a Taylor expansion to fit the parameters in their model. In terms of Eq. (2.51), their parameters correspond to $a_0 = 2a_1 = 4a_2 = C_w$ and $a_3 = 0$. The models in Eqs. (2.50) and (2.51) differ only in how fast the wall pressure grows when $|\mathbf{x} - \mathbf{x}_w| < d_b$. Note that due to the wall force the bubble-volume fraction will be zero at the wall Antal et al. (1991). As a consequence, the wall-tangential components of the bubble velocity cannot be specified at the wall since the bubble-phase deviatoric stress tensor will be zero there (i.e., the bubble phase is inviscid at the wall).

### 2.1.2.7 Bubble-pressure force $\mathbf{F}_{mBP}$

The bubble-pressure force is an interfacial force that models hydrodynamic interactions at the bubble surface:

$$\mathbf{F}_{BP} = -C_{bp}^* \frac{\xi}{\rho_b} (\nabla p_b - \nabla \cdot \mathbf{\tau}_l^\dagger), \quad (2.52)$$

where $p_b$ is the bubble pressure defined by Eq. (2.4) with $C_{bp} \approx 2$, and $\mathbf{\tau}_l^\dagger$ is the part of the liquid-phase shear stress for which the effective viscosity in Eq. (2.15) depends on $\nu_b$. The model parameter $C_{bp}^*$ represents the relative magnitude of the liquid-phase normal stress evaluated at the interface between the bubble and liquid. This parameter is likely to depend on $\epsilon_b$. However, $C_{bp}^* = 1$ when the bubble surface is subject to the same liquid velocity fluctuations as the liquid phase, which we will use as the default value.
2.1.2.8 Bubble coalescence model

One of the primary benefits to using quadrature methods is that the interaction between bubbles can be modeled naturally. When bubbles collide they can coalesce, which leads to a change of the bubble size, and, therefore, of the velocities of bubbles and of other characteristics of the flow. The coalescence rate can be described as the product of a coalescence frequency \( f_{i,j} \) multiplied by an efficiency \( \eta_{i,j} \) Coulaloglou and Tavlarides (1977).

\[
C_c(d_{\alpha_1}, d_{\alpha_2}) = f(d_{\alpha_1}, d_{\alpha_2}) \eta(d_{\alpha_1}, d_{\alpha_2}),
\]

(2.53)

where \( d_{\alpha_1} \) and \( d_{\alpha_2} \) are the diameters of the two colliding bubbles. Both of these terms are dependent on the interaction of two bubble sizes. The most common coalescence model was developed by Coulaloglou and Tavlarides (1977) and uses a collisional frequency based on the collision of bubbles due to turbulent fluctuations in the liquid phase, and a coalescence efficiency based to the ratio of drainage time scales between two bubbles and the turbulent time scales.

\[
f(d_{\alpha_1}, d_{\alpha_2}) = C_1 \frac{\epsilon_1^{1/3}}{d_{\alpha_1} + d_{\alpha_2}}^{2} \left( d_{\alpha_1}^{2/3} + d_{\alpha_2}^{2/3} \right)^{1/2},
\]

(2.54)

\[
\eta(d_{\alpha_1}, d_{\alpha_2}) = \exp \left( -C_2 \sqrt{\frac{2 \rho \epsilon_1^{2/3}}{\sigma} \frac{d_{\alpha_1} d_{\alpha_2}}{d_{\alpha_1} + d_{\alpha_2}}} \right),
\]

(2.55)

where \( C_1 \) and \( C_2 \) are model constants, and are usually chosen equal to 0.88 and 6.0·10^9, respectively. While not shown in this paper, any model for coalescence frequency or efficiency can be used with this method Chesters (1991); Prince and Blanch (1990); Sungkorn et al. (2012); Bizmark et al. (2012).

2.1.2.9 Bubble breakup \( C_b \)

The breakup of bubbles is typically determined by the turbulent intensity of the flow around the bubbles. It is assumed that turbulent eddies hit the bubbles and cause breakup. The corresponding model developed by Alopaeus et al. (2006) is

\[
C_b(d_{\alpha_1}) = C_3 \epsilon_1^{1/3} \text{erfc} \sqrt{\frac{C_4}{\rho_1 \epsilon_1^{2/3} d_{\alpha_1}^{5/3}} + C_5 \frac{\mu_1}{\sqrt{\rho_1 \rho_b \epsilon_1^{1/3} d_{\alpha_1}^{4/3}}}},
\]

(2.56)
where $C_3 = 6.0$, $C_4 = 0.04$, and $C_5 = 0.01$ for air-water mixtures. The number and size of bubbles created from the breakup of a bubble is determined by a daughter distribution. Here, a uniform distribution is used:

$$b(p, \xi_{\alpha_1}) = \frac{6}{p+3}\xi_{\alpha_1}^p,$$

(2.57)

with $p$ as the moment order in the size direction and $\xi_{\alpha}$ is the mass of a bubble. The complete breakup integral used to compute the change in bubble size can be seen in Eq. (2.78) and Eq. (2.80).

As with the coalescence kernel, this method is not limited to a single breakup model, and any using the same form can be employed Laakkonen et al. (2006); Luo and Svendsen (1996).

### 2.1.3 QBMM Closure for Polydisperse Bubbly Flow

In this work, the NDF is reconstructed using QBMM Vikas et al. (2011); Yuan et al. (2014). Approximating the NDF with a weighted summation of Dirac delta distributions

$$n(\xi) = \sum_{\alpha=0}^{N-1} w_{\alpha}\delta(\xi - \xi_{\alpha}),$$

(2.58)

where the $N$ weights $w_{\alpha}$ and $N$ abscissas $\xi_{\alpha}$ are computed from the moments $M_p$ with $p \in \{0, 1, 2, \ldots, 2\N - 1\}$ using the Wheeler algorithm Wheeler (1974). Gaussian quadrature is used here, however the Gauss–Radau quadrature is often an attractive alternative in which one abscissa is fixed at a lower bound. The use of the Gauss–Radau quadrature allows the preservation of one additional moment as well as preventing abscissae from becoming too small (not an observed problem, but an extra safeguard). The extended quadrature method of moments (EQMOM) Yuan et al. (2012, 2014), which uses smooth kernel density functions to approximate the NDF, can be used for post-processing to reconstruct the bubble size distributions for the solved moment set. Like Gauss–Radau quadrature, it also uses $2\N + 1$ moments.

The bubble velocity for node $\alpha$, $U_{\alpha}$, is found from $U_p$ using the condiditional quadrature method of moments (CQMOM) Yuan and Fox (2011). Formally, this is done by solving the following set
of linear systems:
\[
\begin{bmatrix}
1 & 1 & \ldots & 1 \\
\xi_0 & \xi_1 & \ldots & \xi_N \\
\vdots & \vdots & \ddots & \vdots \\
\xi_0^{N-1} & \xi_1^{N-1} & \ldots & \xi_N^{N-1}
\end{bmatrix}
\begin{bmatrix}
w_0 \\
w_1 \\
\vdots \\
w_{N-1}
\end{bmatrix}
= 
\begin{bmatrix}
\mathbf{u}_0 \\
\mathbf{u}_1 \\
\vdots \\
\mathbf{u}_{N-1}
\end{bmatrix},
\tag{2.59}
\]
or
\[
[
\mathbf{V}
\]
\cdot
\begin{bmatrix}
\mathbf{R}
\end{bmatrix}
\cdot
\begin{bmatrix}
\mathbf{U}_\alpha
\end{bmatrix}
= 
\begin{bmatrix}
\mathbf{U}_\alpha
\end{bmatrix},
\tag{2.60}
\]
which follows from the definition of \( \mathbf{U}_p \). The solution for the nodal velocities, \( \mathbf{U}_\alpha \), comes from solving
\[
\begin{bmatrix}
\mathbf{u}_0 \\
\mathbf{u}_1 \\
\vdots \\
\mathbf{u}_{N-1}
\end{bmatrix}
= 
\begin{bmatrix}
\begin{bmatrix}
M_0 \\
M_1 \\
\vdots \\
M_{2N-1}
\end{bmatrix}
\end{bmatrix}
\begin{bmatrix}
1 & 1 & \ldots & 1 \\
\xi_0 & \xi_1 & \ldots & \xi_N \\
\vdots & \vdots & \ddots & \vdots \\
\xi_0^{2N-1} & \xi_1^{2N-1} & \ldots & \xi_N^{2N-1}
\end{bmatrix}
\begin{bmatrix}
w_0 \\
w_1 \\
\vdots \\
w_N
\end{bmatrix},
\tag{2.62}
\]
but this nonlinear relation is not useful for computing the weights and abscissas from the moments.
In practice, the Gauss quadrature algorithm uses \( \mathbf{M}_p \) to find \((w_\alpha, \xi_\alpha)\), and then Eq. (2.59) is used to find \( \mathbf{U}_\alpha \).

### 2.1.3.1 Coupling terms

Using the expression of the approximated joint mass–velocity NDF in Eq. (4.4), closure of the coupling term is obtained. For simplicity, we shall assume that \( \rho_b \) is constant, but this is not required Yuan et al. (2014). The bubble-phase volume fraction is then
\[
\varepsilon_b = \frac{1}{\rho_b} \int_0^\infty \xi n(\xi) \, d\xi = \frac{M_1}{\rho_b}.
\tag{2.63}
\]
The coupling term due to momentum exchange between the two phases in Eq. (2.13) is

$$M_{lb} = - \int_0^\infty F_{lb} n(\xi) \, d\xi,$$  \hspace{1cm} (2.64)

where $F_{lb}$ is the sum of interfacial forces acting on the bubbles:

$$F_{lb} = F^B + F^D + F^{VM} + F^L + F^W + F^{BP}.$$  \hspace{1cm} (2.65)

Note that while some force terms in Eq. (2.64) can be expressed in closed form, due to the dependence on $\xi$ of the coefficients, most of the terms require the knowledge of $n(\xi)$.

Gauss quadrature weights and abscissae for each node are related to the gas density and volume fraction by $w_\alpha \xi_\alpha = \rho_b \varepsilon_\alpha$ where $\varepsilon_b = \sum_{\alpha=0}^{N-1} \varepsilon_\alpha$ (see Eq. (2.63)). From Eq. (2.64), we define

$$M_{lb} = - \sum_{\alpha=0}^{N-1} w_\alpha F_{lb,\alpha},$$  \hspace{1cm} (2.66)

where $F_{lb,\alpha}$ denotes the forces defined in Sec. 2.1.2, evaluated at $\xi = \xi_\alpha$. For completeness, the individual forces are given in Table 2.1, where $U_\alpha$ is the bubble velocity for node $\alpha$. The coefficients of the interfacial force terms depend on $\alpha$ through the bubble diameter $d_\alpha = (6\xi_\alpha/\pi \rho_b)^{1/3}$ and $U_\alpha$.

### 2.1.3.2 Monodisperse bubbly flow model

In the monodisperse limit, $\rho_b \varepsilon_b = N \xi_b = M_1$ where $N = M_0$ is the number density of bubbles. In this limit, Eq. (2.29) yields the bubble-phase continuity equation:

$$\frac{\partial \rho_b \varepsilon_b}{\partial t} + \nabla \cdot (\rho_b \varepsilon_b U_b) = 0.$$  \hspace{1cm} (2.67)
Likewise, Eq. (2.30) with $p = 1$ yields the bubble-phase momentum equation:

$$\frac{\partial \rho_b \varepsilon_b U_b}{\partial t} + \nabla \cdot \left( \rho_b \varepsilon_b U_b \otimes U_b + p_c I - \tau_c \right) = \rho_b \varepsilon_b g - M_{lb}. \quad (2.68)$$

In the complete two-fluid model, the bubble-phase balances in Eq. (2.67) and Eq. (2.68) are coupled to the liquid-phase balances given in Eq. (2.12) and Eq. (2.13). The final form of the momentum coupling term for monodisperse bubbly flow is

$$M_{lb} = \varepsilon_b \left[ \nabla (p_l + p_b + p_w) - \nabla \cdot \tau_l \right] + K_{\text{drag}} \left[ \varepsilon_b (U_b - U_l) + \frac{\delta_{\text{dis}}}{\varepsilon_1} \nabla \varepsilon_b \right]$$

$$+ \varepsilon_b \rho_l C_{\text{vm}} \frac{D}{Dt} (U_b - U_l) - \varepsilon_b^2 \rho_l (U_b - U_l) \nabla \cdot U_b$$

$$+ \varepsilon_b C_L \rho_l (U_b - U_l) \times (\nabla \times U_l), \quad (2.69)$$

where the convective time derivative of the velocity difference is defined by

$$\frac{D}{Dt} (U_b - U_l) = \frac{\partial}{\partial t} (U_b - U_l) + U_b \cdot \nabla (U_b - U_l). \quad (2.70)$$

### 2.1.3.3 Polydisperse bubbly flow model

For polydisperse bubbly flow, Eq. (2.67) is replaced by continuity relations for the size moments found from Eq. (2.25):

$$\frac{\partial N}{\partial t} + \nabla \cdot \left( \int_0^\infty U(\xi)n(\xi) \, d\xi \right) = C_0, \quad (2.71)$$

$$\frac{\partial \rho_b \varepsilon_b}{\partial t} + \nabla \cdot (\rho_b \varepsilon_b U_b) = 0, \quad (2.72)$$

and for $1 < p \leq 2N - 1$:

$$\frac{\partial M_p}{\partial t} + \nabla \cdot \left( \int_0^\infty \xi^p U(\xi)n(\xi) \, d\xi \right) = C_p, \quad (2.73)$$

where $C_p$ is the change due to coalescence and breakage. Here, Eq. (2.72) is due to conservation of mass and the definition of the mean bubble velocity:

$$\varepsilon_b \rho_b U_b = \int_0^\infty \xi U(\xi)n(\xi) \, d\xi. \quad (2.74)$$
The spatial fluxes in Eqs. (2.71)-(2.73) depend on the reconstruction of the size NDF. The spatial flux for $M_p$ is found from

$$U_p = \int_0^\infty \xi^p U(\xi) n(\xi) \, d\xi = \sum_{\alpha=0}^{N-1} w_\alpha \xi_p^0 U_\alpha.$$  \hspace{1cm} (2.75)

The moment conservation equation

$$\frac{\partial M_p}{\partial t} + \nabla \cdot U_p = C_p \quad \text{for } p \in \{0, 1, \ldots, 2N - 1\}$$  \hspace{1cm} (2.76)

is thus coupled to Eq. (2.30) through the definition of the spatial fluxes in Eq. (2.74). The entire conservative system of the $N$ bubble pseudo-phases, or number of discrete bubble sizes used to approximated the bubble size distribution, and the liquid phase can be solved using finite-volume methods as described in Sec. 2.1.4.

2.1.3.4 Coalescence and breakage terms

The source term used to account for size change is broken into two parts, the first to account for the birth of bubbles ($B^c_p$ and $B^b_p$), and the second for the death of bubbles ($D^c_p$ and $D^b_p$):

$$B^c_{p,i,j,k} = \frac{1}{2} \sum_{\alpha_1}^{N-1} w_{\alpha_1} v^i_{x,\alpha_1} v^j_{y,\alpha_1} v^k_{z,\alpha_1} \sum_{\alpha_2}^{N-1} w_{\alpha_2} \left( \xi_{\alpha_1} + \xi_{\alpha_2} \right)^p C_c(d_{\alpha_1}, d_{\alpha_2}),$$  \hspace{1cm} (2.77)

$$B^b_{p,i,j,k} = \sum_{\alpha_1}^{N-1} w_{\alpha_1} v^i_{x,\alpha_1} v^j_{y,\alpha_1} v^k_{z,\alpha_1} C_b(d_{\alpha_1}) \bar{b}(p, \xi_{\alpha_1}),$$  \hspace{1cm} (2.78)

$$D^c_{p,i,j,k} = \frac{1}{2} \sum_{\alpha_1}^{N-1} w_{\alpha_1} v^i_{x,\alpha_1} v^j_{y,\alpha_1} v^k_{z,\alpha_1} \sum_{\alpha_2}^{N-1} w_{\alpha_2} \left( \xi^p_{\alpha_1} + \xi^p_{\alpha_2} \right) C_c(d_{\alpha_1}, d_{\alpha_2}),$$  \hspace{1cm} (2.79)

$$D^b_{p,i,j,k} = \sum_{\alpha_1}^{N-1} w_{\alpha_1} v^i_{x,\alpha_1} v^j_{y,\alpha_1} v^k_{z,\alpha_1} \xi^p_{\alpha_1} C_b(d_{\alpha_1}).$$  \hspace{1cm} (2.80)

In these equations, $N$ is the number of nodes, $C_c(d_{\alpha_1}, d_{\alpha_2})$ and $C_b(d_{\alpha_1})$ are computed from the chosen coalescence and breakup models, and $\bar{b}(p, \xi_{\alpha_1})$ is the specified daughter distribution. After combining all birth and death terms, the final form of the source terms accounting for bubble size
change is:

\[
C_{p,i,j,k} = C_{c,p,i,j,k} + C_{b,p,i,j,k} = B_{p,i,j,k}^c - D_{p,i,j,k}^c + B_{p,i,j,k}^b - D_{p,i,j,k}^b \\
= \frac{1}{2} \sum_{\alpha_1}^N w_{\alpha_1} v_{x,\alpha_1} v_{y,\alpha_1} v_{z,\alpha_1} \sum_{\alpha_2}^N w_{\alpha_2} C_c(d_{\alpha_1}, d_{\alpha_2}) \\
\times \left[ (\xi_{\alpha_1} + \xi_{\alpha_2})^p - (\xi_{\alpha_1}^p + \xi_{\alpha_2}^p) \right] \\
+ \sum_{\alpha_1}^N w_{\alpha_1} v_{x,\alpha_1} v_{y,\alpha_1} v_{z,\alpha_1} C_b(d_{\alpha_1}) (\xi_{\alpha_1}^p - b(p,\xi_{\alpha_1})). \tag{2.81}
\]

In the numerical algorithm, the coalescence and breakage terms are handled separately from spatial transport using operator splitting.

### 2.1.4 Numerical Algorithm for Polydisperse Bubbly Flow

The numerical algorithm for the solution of the bubbly flow needs to be capable of managing both the cases of a flow with high gas volume fraction and of complete absence of disperse phase. The dense regime in which bubbles are highly concentrated, is characterized by all bubbles moving with the same velocity \( M_p U_b = U_p \). In this regime, the convective fluxes in Eq. (2.31) reduce to \( \mathcal{P}_p = M_p U_b \otimes U_b \), i.e., all size moments have the same characteristic velocity. Near the dense limit, the bubble-phase momentum balance reduces to

\[
\frac{\partial M_1 U_b}{\partial t} + \nabla \cdot \left( M_1 U_b \otimes U_b + \mathcal{P}_{1,v} \right) = M_1 g + M_1 \tilde{A} - \tilde{D}_{\text{dis}} \nabla M_1, \tag{2.82}
\]

where the mass-averaged terms \( \tilde{A} \) and \( \tilde{D}_{\text{dis}} \) depend on \( U_b \), and \( \mathcal{P}_{1,v} \) is a pressure tensor arising due to polydispersity. When all bubble sizes have the same velocity, \( \mathcal{P}_{1,v} \) is null.

By splitting the convective fluxes as described in Sec. 2.1.1.4, Eq. (2.29) and Eq. (2.30) yield

\[
\frac{\partial M_p}{\partial t} + \nabla \cdot \mathcal{V}_p + \nabla \cdot M_p U_b = \mathcal{C}_p, \tag{2.83}
\]

and

\[
\frac{\partial U_p}{\partial t} + \nabla \cdot \mathcal{P}_{p,v} + \nabla \cdot \mathcal{P}_{p,b} \\
= M_p g + \int_0^{\infty} \xi^p \left( \mathcal{A} - D_{\text{dis}} \nabla \ln n(\xi) \right) n(\xi) d\xi - \frac{\xi_b g_0}{\tau_c} \mathcal{V}_p + \mathcal{C}_p. \tag{2.84}
\]
With \( p = 1 \), we have \( V_1 = 0 \), \( P_{p,b} = M_1 U_b \otimes U_b \) and \( U_1 = M_1 U_b \), so that Eq. (2.83) and Eq. (2.84) can be solved with a standard two-fluid solver for bubbly flow. From a numerical perspective, the fluxes involving \( V \) can be treated using a kinetic-based scheme and operator splitting. This leads to the following algorithm:

1. Given the cell-average \( M_p \) and \( U_p \),\(^1\) use the multivariate moment-inversion algorithm described in Sec. 2.1.3 to find \( w_\alpha, \xi_\alpha \) and \( U_\alpha \) for the bubbly phase. By definition, the velocity of bubbles with size \( \xi_\alpha \) with respect to the mean, at cell centers, is \( V_\alpha = U_\alpha - U_b \). Using numerical quadrature we have

\[
V_p = \sum_\alpha w_\alpha \xi_\alpha V_\alpha,
\]

and

\[
P_{p,v} = \sum_\alpha w_\alpha \xi_\alpha V_\alpha \otimes U_\alpha.
\]

2. Use a kinetic-based advection scheme Perthame (1992); Marchisio and Fox (2013) to partially update \( M_p \) and \( U_p \) for all \( p \) from

\[
\frac{\partial M_p}{\partial t} + \nabla \cdot V_p = 0,
\]

and

\[
\frac{\partial U_p}{\partial t} + \nabla \cdot P_{p,v} = 0.
\]

Here the kinetic fluxes are based on \( V_\alpha \) using a uniform spatial reconstruction (i.e., the abscissas are constant in each cell). Applying Gauss’ theorem to the divergence term of the integral form of Eq. (2.86) and Eq. (2.87) leads to

\[
\int_\Omega \nabla \cdot V_p \, dS = \sum_f \sum_\alpha \left[ w_{\alpha,\text{own}} \xi_{\alpha,\text{own}} \max \left( V_{\alpha,\text{own}} \cdot S_f, 0 \right) 
+ w_{\alpha,\text{nei}} \xi_{\alpha,\text{nei}} \min \left( V_{\alpha,\text{nei}} \cdot S_f, 0 \right) \right],
\]

\(^1\)Initial values of the moments are computed based on the input variables, which are the phase individual volume fractions \( \varepsilon_\alpha \), the phase densities, the bubble size of each bubble class \( d_{b,\alpha} \), and the bubble velocities \( U_\alpha \). The only quantities which need to be calculated before proceeding with the computation of the initial moments are the quadrature weights:

\[
w_\alpha = \frac{6 \varepsilon_\alpha}{\pi d_{b,\alpha}^3}
\]
\begin{equation}
\int_{\Omega} \nabla \cdot p_{p,v} \, dS = \sum_f \sum_{\alpha} \left[ w_{\alpha,own} e_{\alpha,own} U_{\alpha,own} \max (V_{\alpha,own} \cdot S_f, 0) \\
+ w_{\alpha,nei} e_{\alpha,nei} U_{\alpha,nei} \min (V_{\alpha,nei} \cdot S_f, 0) \right]
\end{equation}

(2.89)

where the index \( f \) iterates over the cell faces, and the subscripts \textit{own} and \textit{nei} represent the reconstructed values at cell faces based on the cell owner and neighbor of the face, respectively.

Note that \( M_1 \) (and, hence, \( \varepsilon_b \)) should remain unchanged in this step, but any numerical errors will be corrected in step 5. The moments, \( M_p^* \) and \( U_p^* \), are partially updated and will be realizable if a realizable scheme is used to evaluate the weights \( w_\alpha \) at the cell interfaces.

3. Given the cell-average \( M_p^* \) and \( U_p^* \), use the moment-inversion algorithm to recompute \( w_\alpha, \xi_\alpha, \) \( U_\alpha \) and \( V_\alpha \). Note that the cell-average velocity \( U_b = U_1^*/M_1 \) may change in Step 2. As a consequence, the fluxes that are function of \( U_b \), including the total flux, need to be updated before starting to solve the two-fluid equations at the next step.

4. Given the current \( M_1 = \rho_b \varepsilon_b \) and \( U_1 = \rho_b \varepsilon_b U_b \), use a two-fluid solver to update \( M_1 \) and \( U_1 \), and fluid-phase \( \varepsilon_l, \varepsilon_l U_l \). This is done using

\begin{equation}
\frac{\partial \rho_b \varepsilon_b}{\partial t} + \nabla \cdot \rho_b \varepsilon_b U_b = 0,
\end{equation}

(2.90)

\begin{equation}
\frac{\partial \rho_b \varepsilon_b U_b}{\partial t} + \nabla \cdot \left[ \rho_b \varepsilon_b U_b \otimes U_b + p_b I - \tau_c \right]
= \int_0^\infty \xi \left( A - D_{\text{dis}} \nabla \ln n(\xi) \right) n(\xi) \, d\xi,
\end{equation}

(2.91)

and flux limiters may be needed to ensure that \( 0 \leq \varepsilon_b \leq 1 \). Denote the flux-limited bubble velocity by \( U_b^\text{f} \) (i.e., the cell-face values of bubble velocity), which will be needed in the next step. The integral term in Eq. (2.91) is evaluated using numerical quadrature. In order to provide more details concerning the implementation, the terms of this integral are examined separately:
• Buoyancy force

The contribution to the integral in Eq. (2.91) is

\[
\int_{0}^{+\infty} \xi n(\xi) \frac{\nabla \cdot \tau^*_i - \nabla p_l}{\rho_b} d\xi = \sum_{\alpha} w_{\alpha} \xi_{\alpha} \frac{\rho_{\alpha}}{\rho_b} (\nabla \cdot \tau^*_1 - \nabla p_l) = \varepsilon_b (\nabla \cdot \tau^*_1 - \nabla p_l) \quad (2.92)
\]

Because the pressure and stress tensor do not depend on \( \xi \), and the term \( \sum_{\alpha} w_{\alpha} \xi_{\alpha} / \rho_b \) is the total volume fraction. In the solution of the two-fluid model, the pressure gradient is removed in the construction of the mean momentum equations, and its contribution is later accounted for through the pressure correction found from the solution to the pressure equation. It should also be noted that in the solution of velocity abscissae, the corresponding size volume fraction is used, not the total bubble phase volume fraction.

• Drag force

The implementation of the drag force requires care to ensure the robustness of the iterative solution procedure. We observe that

\[
\mathcal{D}^\text{drag} = \int_{0}^{+\infty} \xi n(\xi) \frac{K^\text{drag}}{\rho_b} (U_l - U) d\xi = \sum_{\alpha} w_{\alpha} \xi_{\alpha} \frac{K^\text{drag}(U_{\alpha}, d_{b,\alpha})}{\rho_b} (U_l - U_{\alpha}). \quad (2.93)
\]

This expression does not explicitly depend on the mean gas velocity \( U_b \), which is needed to have a partially implicit treatment of the drag term in two-fluid iterative solver. However, it can be observed that \( U_{\alpha} = V_{\alpha} + U_b \), where \( V_{\alpha} \) is updated before Step 4 is started. Substituting this into Eq. (2.93) leads to:

\[
\mathcal{D}^\text{drag} = \sum_{\alpha} w_{\alpha} \xi_{\alpha} \frac{K^\text{drag}(U_{\alpha}, d_{b,\alpha})}{\rho_b} (U_l - U_{\alpha}) - \sum_{\alpha} w_{\alpha} \xi_{\alpha} \frac{K^\text{drag}(U_{\alpha}, d_{b,\alpha})}{\rho_b} V_{\alpha}. \quad (2.94)
\]

The first term of the summation on the right-hand side of Eq. (2.94) can now be treated as conventionally done in two-fluid solvers, observing that the coefficient multiplying the
slip velocity is replaced by the summation \( \sum_{\alpha} w_{\alpha} \xi_{\alpha} K_{\text{drag}}(U_{\alpha})/\rho_b \). The second term can be included in the flux used to define the pressure equation.

• Lift force

The lift force does not present particular difficulty, since it is treated explicitly or as a flux in two-fluid algorithms. The corresponding integrated term is

\[
\int_0^{+\infty} \xi n(\xi) \frac{C_L \rho_l}{\rho_b} (U_1 - U) \times (\nabla \times U_1) \, d\xi = \sum_{\alpha} w_{\alpha} \xi_{\alpha} C_{L,\alpha} \frac{\rho_l}{\rho_b} (U_1 - U_{\alpha}) \times (\nabla \times U_1). \tag{2.95}
\]

Note that, if the lift coefficient is not constant, it may depend on the quadrature abscissae.

The same approach used for the lift force can be used for the wall-lubrication force, the expression of the integral of which is omitted for brevity.

• Dispersion force

While \( D_{\text{dis}} \) is a function of the volume fraction, it is assumed to be independent from \( \xi \) (the mass). Hence, each bubble size has a unique \( D_{\text{dis},\alpha} \). The integrated term for the dispersion force is

\[
D_{\text{dis}}(\xi) = - \int_0^{+\infty} \xi n(\xi) \frac{\rho_l}{\rho_b} D_{\text{dis}} \nabla \ln \xi \, d\xi = - \sum_{\alpha} D_{\text{dis},\alpha} \nabla \left( \frac{w_{\alpha} \xi_{\alpha}}{\rho_l} \right). \tag{2.96}
\]

• Virtual-mass force

The integrated contribution of the virtual-mass force is given by

\[
D_{\text{VM}} = \int_0^{+\infty} \xi n(\xi) \rho_l C_{\text{VM}} \left( \frac{dU_1}{dt} - \frac{dU}{dt} \right) \, d\xi. \tag{2.97}
\]
In order to treat the virtual mass implicitly, as is typically done, the source term is split into mean and deviation terms (similar to drag):

\[
\mathbb{D}_\text{VM} = \sum_\alpha w_\alpha \xi_\alpha C_{\text{VM, } \alpha} \frac{\rho_\alpha}{\rho_b} \times \left[ \left( \frac{dU_\alpha}{dt} - \frac{dU_b}{dt} \right) - \left( \frac{dU_\alpha}{dt} - \frac{dU_b}{dt} \right) \right],
\]

(2.98)

where the mean is used in the momentum equation and the deviation is added into the flux included in the pressure equation. It is noted that \( C_{\text{VM}} \) can be a function of the bubble size.

5. Because the phase volume fraction flux, \((\varepsilon \phi)_b\), is limited in the two fluid model and not the volumetric flux, \(\phi_1^\dagger\), which is used to advect the moments, differences between \(M_1\) and \(\varepsilon_b \rho_b\) are observed. A correction term is added to \(\phi_1^\dagger\) so that \(M_1\) is made consistent with the two fluid model, addressing this inconsistency. The correction term, \(\psi\) is determined from

\[
\frac{\alpha_b \rho_b - M_1^*}{\Delta t} + \nabla \cdot (M_1^* U_b) + \nabla \cdot (M_1^* \nabla \psi) = 0,
\]

(2.99)

where \(\alpha_b \rho_b\) is the weighted mass of the bubble phase after the two fluid model is solved, \(M_1^*\) is the size moment of order one after being transported with the deviation fluxes, and \(\phi_1^\dagger\) is the limited flux from the two fluid model. The mean flux is then corrected with

\[
\phi_1^* = \phi_1^\dagger + |S_f| \nabla \cdot (\psi) f.
\]

(2.100)

Zero gradient boundary conditions are used everywhere except for one boundary where a fixed value is used to set a reference level for \(\psi\). This fixed value should be set at a boundary where there is only air so only a mean velocity exists, hence no correction is needed because this is the total volumetric flux and is correct.

6. Starting from the cell-average \(M_p^*\) and \(U_p^*\), finish updating \(M_p\) and \(U_p\) by solving

\[
\frac{\partial M_p}{\partial t} + \nabla \cdot M_p U_p^* = 0
\]

(2.101)
and

\[ \frac{\partial U_p}{\partial t} + \nabla \cdot \mathcal{P}^*_p = M_p \mathbf{g} + \int_0^\infty \xi^p (A - D_{\text{dis}} \nabla \ln n(\xi)) n(\xi) \, d\xi + \frac{\varepsilon_b g_0}{\tau_c} (M_p \mathbf{U}_b - U_p), \quad (2.102) \]

where \( \mathcal{P}^*_p = \mathbf{U}_b^* \otimes \mathbf{U}_p \). As the advection velocity \( \mathbf{U}_b^* \) is independent of \( \xi \), a realizable kinetic-based scheme can be used for the advection terms \( M_p \mathbf{U}_b^* \) and \( \mathcal{P}^*_p \). For this purpose, advection can be treated separately using operator splitting. For consistency, \( M_p \) in the collisional flux should be reconstructed at the cell faces using the cell-average abscissas \( \xi_\alpha \) and face-value weights \( w_\alpha \). The solution of Eq. (2.102) can be achieved with a splitting procedure, in the following order:

- Advection with only the kinetic fluxes, computed with a kinetic scheme, in which the advection velocity is represented by the mean bubble velocity \( \mathbf{U}_b^* \) in a manner similar to Eq. (2.88) and Eq. (2.89). The only difference is that since \( \mathbf{U}_b^* \) is independent of \( \xi \), the flux can be taken out of the summation.

- Because the change in bubble momentum due to interfacial forces is independent of \( \xi \), \( N \) equations for the size-dependent bubble velocities can be solved to account for the change in velocities due to interfacial forces and bubble–bubble interactions:

\[ w_\alpha \xi_\alpha \frac{\partial \mathbf{U}_\alpha}{\partial t} = w_\alpha \xi_\alpha \mathbf{g} + \mathbf{M}_{b,\alpha} \]

\[ - D_{\text{dis,}\alpha} \nabla \left( \frac{w_\alpha \xi_\alpha}{\rho_b} \right) + \frac{w_\alpha \xi_\alpha g_0}{\tau_c} (\mathbf{U}_b - \mathbf{U}_\alpha). \quad (2.103) \]

7. After the final solution of Eq. (2.103), the velocity moments are recomputed using Eq. (2.59). Additionally, the mean velocity, \( \mathbf{U}_b \) and mean flux \( \phi_b \) are updated using \( \mathbf{U}_b = \mathbf{U}_1 / M_1 \) and \( \phi_b = (\mathbf{U}_b)_f \cdot \mathbf{S}_f \) where \((\mathbf{U}_b)_f\) is the interpolated bubble phase velocity.

8. Lastly, the effect of bubble coalescence and breakup is accounted for by solving the ODEs for the change in the size and velocity moments using

\[ \frac{\partial M_p}{\partial t} = \mathcal{C}_p, \quad (2.104) \]
and
\[ \frac{\partial U_p}{\partial t} = C_p. \]  

(2.105)

The coupling between the size and velocity moments is important because the velocity nodes do not remain constant though this step, instead they will change to ensure that momentum of the bubble phase is conserved. The source breakup and coalescence kernels can also depend on the relative velocity between bubble sizes (Lehr and Mewes, 2001), meaning that this source terms needs to be updated after every sub-step. This system is solved using the RK2-SSP with adaptive time stepping described in Nguyen et al. (2016). It should be noted that mass and momentum are conserved in this step so the first order moments do not change.

9. Return to Step 1 with updated \( M_p \) and \( U_p \).

2.1.5 Applications

The method proposed in the previous sections is here applied to a series of test cases to investigate its mathematical behavior and to illustrate its application to relevant problems involving bubbly flows. First the mathematical properties of the model are studied by performing grid refinement in a case with and segregated bubble-size distribution to show that the model is hyperbolic and has the ability to handle the evolution from segregated bubble sizes to conditions when different sizes co-exists in the same discretization volume. The behavior of the model in the monodisperse limit is then verified against the numerical predictions obtained with the two-fluid solver in OpenFOAM (twoPhaseEulerFoam)(OpenCFD Ltd., 2018). The predictions of the model are validated experimental cases considering both the bubble column with a central injection, described in Pfleger et al. (1999), and the experimental data of Díaz et al. (2008). As a last step, the ability of the model to handle flows in complex geometries, discretized with an triangular grid, and involving coalescence and breakup, is examined in a two-phase system with high injection velocity of the gas phase.
2.1.5.1 Mixing of bubbles size distributions

The ability of the approach to handle cases with initially segregated bubble size distributions which mix, while preserving moments and the hyperbolic behavior is shown considering a one-dimensional shock tube. The tube is 1 m long and is discretized with increasing resolutions of 1000, 5000, 10000, and 20000 computational cells. The distribution in the bottom half consists of equal volume fraction of 8, 9, and 10 mm bubbles. The top distribution consists of equal volume fractions of 1, 2, and 3 mm bubbles. The initial volume fraction of the bubble phase is initially uniformly equal to 0.1 throughout the tube. The bottom boundary is a no-slip wall, with Neumann conditions for scalar quantities. The top boundary is set to an outflow condition, ensuring no backflow occurs. Because the larger bubbles have a higher rise velocity, the bubble size distributions, originally represented by Dirac delta distributions, mix and show a change in the mean diameter. This process also causes chaotic behavior around the shock lines of the discrete bubble sizes, as it can be seen in Fig. 2.1.5.1, 2.1.5.1, and 2.1.5.1.

The results show that, while the volume fraction of the domain is initially uniform, allowing multiple distributions of bubble sizes to move through one another causes unexpected dynamics. While spikes are present in results using the higher resolutions, they do not appear to become unbounded with increasing resolution, but instead the results appear to converge to a solution.
Figure 2.2  Bubble vertical velocity

Figure 2.3  Bubble mean diameter
using a grid size of $\Delta x = 0.05$ mm. The areas of very high volume fractions occur where multiple bubble sizes meet in singular point in space and being to move at the same speed due to interactions. This means that the larger bubbles are no longer moving though the smaller bubbles, instead they are reaching an equilibrium velocity. This causes a sudden increase in volume fraction, and gives the results seen in 2.1.5.1. The decrease in velocity in front of the shock is due to the fact that since larger bubbles are no longer moving through the smaller bubbles, the mean rise velocity decreases as existing bubbles in this area are advected higher. A possible reconstruction of the BSD, obtained with the two-node $\Gamma$-EQMOM (Yuan et al., 2012), is shown in Fig. 2.4 for $t = 0.75$. Only two nodes were used because one additional moments is needed for EQMOM reconstruction, and moments for high-order reconstructions are not considered in the proposed approach. The reconstructed distribution in Fig. 2.4 shows the presence of both distributions at a single point, however it should be mentioned that this is only one of the possible NDFs corresponding to the truncated moment vector used to obtain the reconstruction.
2.1.5.2 Monodisperse case

In this section, the solver is verified and validated in the monodisperse limit considering the geometry illustrated in Fig. 2.5 and using the boundary conditions summarized in Table 2.2.

The objective of this effort is to show that the proposed method properly degenerates into a two-fluid model in the monodisperse limit. To such purpose, results predicted with the proposed approach are compared to the solution obtained with the standard two-fluid model available in OpenFOAM. Only drag and buoyancy force are considered here, following Pfleger et al. (1999). The inlet volume fraction and superficial bubble velocity is $\varepsilon_b = 1$ and $0.03 \text{ cm/s}$ respectively. The bubble size is assumed to be 2 mm, and the drag model used is Schiller and Naumann (1933)’s. The results of the QBMM solver and OpenFOAM’s two-phase Eularian solver are presented in Fig. 2.6 and 2.7 respectively.
Figure 2.6 Time-averaged results using a single bubble size with QBMM solver

Figure 2.7 Time-averaged results using the monodisperse two-fluid solver
Figure 2.8  Vertical liquid velocity versus column width

(a) Sampling at height of 0.13 m  
(b) Sampling at height of 0.25 m

(c) Sampling at height of 0.37 m
All the figures show good agreement between results obtained from twoPhaseEulerFoam and QBMM, except for the velocity profiles in areas of low bubble volume fractions. This difference occurs in the limit when the bubble volume fraction is negligible and the drag approaches zero. This discrepancy in bubble velocities may be attributed to the different numerical implementation of the drag force in the QBMM approach compared to the two-fluid model, which is required for the general polydisperse case. The comparison of liquid velocities at three different heights (0.13 m, 0.25 m, and 0.37 m), shown in Fig. 2.8, show good agreement, with little to no deviation between solutions obtained with QBMM and the two-fluid model, except the valleys in velocity at near the walls in which the two solution are mirrored. The time-averaged volume fraction predicted by the two approaches is also identical. These results show that in the monodisperse limit, the first moments of the joint size–velocity NDF are unaffected by the deviation moments, as expected, since the latter are null. The simulation completed with twoPhaseEulerFoam OpenCFD Ltd. (2018a) took 50 min, while the OpenQBMM solver took 65 min, both on a workstation with a dual Intel Xeon CPU Intel® Xeon® CPU E5-2667 v3 at 3.20 GHz, using 4 cores with an adaptive time-step allowing a maximum Courant number of 0.5. This additional time is likely due to the fact that the moments are inverted at each step, as well as to the additional Poisson equation solved each step used to correct the bubble-phase mean flux.

2.1.5.3 Pfleger polydisperse case

The same system described in Pfleger et al. (1999), with the same geometry and boundary conditions as the case in the previous section, is simulated in this section using QBMM and assuming a polydisperse flow with three unique bubble sizes (1 mm, 2.5 mm, and 4 mm), all with equal volume fractions and velocities at the inlet ($\xi_3 w_3 + \rho_b = 0.33$). Using these known values, the mass of a single bubble (the abscissa) was calculated, and the volume fraction was then used to calculate the number of bubbles per unit volume (weight). These quantities were then used to construct the $2N$ moments required by the standard moment inversion. As in the previous case, only drag and buoyancy were used in this simulation.
Simulation results are shown in Fig. 2.9, where they are compared to both experiments and simulations from Pfleger et al. (1999). Fig. 2.10 shows the comparison of QBMM results to the experiments, monodisperse simulations, and multiphase simulations using three bubble phases with constant diameter to represent bubbles of different sizes.

Additionally, a 3-D case was run using QBMM as well to study the effect of the two-dimensional representation of the computational domain on the accuracy of the predictions. It is apparent that two-dimensional simulations are unable to properly predict the velocity profile in the system, while three-dimensional simulations provide the best level of agreement with the experimental data. In addition, the average bubble diameter also shows the expected qualitative distribution of bubbles throughout the domain, where larger bubble are more concentrated at the center of the column with smaller bubbles concentrating further from the center Tomiyama (1998). The cost of the QBMM method was roughly three times that of the multi-fluid fluid simulation (17 h compared to 5 h on 4 CPU cores of the same workstation described before). This is primarily due to the restriction on the Courant number (Co) in order to preserve the realizability of the moment set, QBMM required
Figure 2.10  Vertical liquid velocity versus column width of Pfleger simulations, experiments, and polydisperse simulation
Co = 0.1, while the multi-fluid solver only required Co = 0.5. However when the multi-fluid solver used a Courant number of 0.1, the simulation took 31 hours. It should also be noted that with no breakup or coalescence kernels included, the bubble sizes stay exactly the same through the entire domain.

2.1.5.4 Díaz polydisperse case

The last case used to validate the polydisperse solver is described in Díaz et al. (2008), in which the same geometry is used as in the prior two cases, however the inlet velocity is varied and the plume oscillation time and gas hold-up are observed. The bubble sizes used in this case are 3.5 mm, 5 mm, and 6.5 mm, all equal in volume fraction, with a mean chosen to match experimental observation (5 mm (Díaz et al., 2008)), and the same approach to construct initial moments was used as in the previous example. No information about the size distribution was given from experimental data, so an arbitrary distribution was used. As mentioned previously, all source terms included in Sec. 2.1.2 are used in these simulations. The dispersion coefficient was modeled according to Panicker et al. (2018), drag and lift forces are described by the model of Tomiyama (Tomiyama et al., 1998, 2002), the wall-pressure model of Antal et al. (1991) was used, and a constant virtual-mass coefficient of 0.5 was used.

An example of the averaged fields obtained from the simulations can be seen in Fig. 2.12, while the pressure oscillations in the column as a function of time are reported in Fig. 2.11. It can be seen in Fig. 2.12 that the magnitude and frequency of the low frequency oscillations match very well with that observed in experiments. The difference in the high frequency oscillations is due to experimental noise. While the pressure oscillations show good agreement for the lower flow rates, the plume oscillations for higher inlet velocities are less frequent (roughly half the frequency) than is seen in the experiments, this is likely due to the diffusion added by the first order schemes. The experiments also show visually a near uniform region of bubbles in the upper half of the column something that is not predicted (Fig. 2.12). While this is not seen, the flow regimes are predicted
Figure 2.11 Results obtained in the Díaz case for 1.19 cm/s inlet velocity

Quite well with liquid re-circulation zones along the walls for inlet velocities less than or equal to 2.4 cm/s, and higher velocities beginning to drag bubbles into these vorticies.

2.1.5.5 Mixing vessel on unstructured mesh

The final case used to test the solver was selected to demonstrate the capability of the approach to deal with complex geometries discretized using triangular grids. In addition, it shows the ability of the method to handle difficult case setups, with high superficial velocity, as well as the ability to account for breakup and coalescence. The geometry of a mixing vessel was selected due to its common presence in industrial applications. A close up of the inlet section (bottom of the mixer) can be seen in Fig. 2.13(a) and the mesh, consisting of 6232 cells can be seen in Fig. 2.13(b). The inlet diameter is 1 cm and the outer mixer diameter is 1 m. The height of the angled section is 1 m and an initial water height of 2.7 m was used. The superficial inlet gas velocity is 10 m/s, and a gas volume fraction of 1.0. The coalescence and breakup described in Secs. 2.1.2.9 and 2.1.2.8 are used in this application. The turbulent time-scale necessary for the coalescence and breakup
Figure 2.12 Normalized pressure at different inlet velocities in Díaz case
closure models was obtained using the Smagorinsky (1963) eddy viscosity model. The same drag, virtual mass, and lift models were used as in Sec. 2.1.5.4.

The simulation was run for 25 s of actual flow time. Results at 2 s and 25 s can be seen in Figs. 2.14 and 2.15. The bubble size distribution at the center of the vessel, 1 m vertically from the inlet (can be seen in the contour plots of bubble diameter), at \( t = 2 \) s and \( t = 25 \) s, has been reconstructed using the two-node Γ-EQMOM, and can be seen in Fig. 2.16.

2.1.6 Conclusions

A quadrature-based algorithm to simulate polydisperse bubbly flows with evolving size distribution was presented. A robust computational method was formulated in order to ensure the stability of the solution of the model in cases where the gas phase is highly concentrated or absent. An example application was considered to demonstrate that the approach properly degenerates into a two-fluid model in the mono-disperse limit. The predictive capabilities of the approach were then verified considering the bubble column of Pfleger et al. (1999) and of Díaz et al. (2008). Good agree-
Figure 2.14 Instantaneous fields at $t = 2$ s.

Figure 2.15 Instantaneous fields at $t = 25$ s.
Figure 2.16  Example of the bubble size distribution reconstructed using gamma-EQMOM at the center of the vessel.
ment was observed when three-dimensional simulations are used for the first case. The QBMM approach predicted pressure oscillation in agreement with experiments from Díaz et al. (2008). However, like the standard two-fluid model, the gas hold-up was significantly under-estimated at high gas flow rates. Lastly, the capability of the approach to be used to simulate bubbly flows with coalescence and breakage in non-trivial geometries was demonstrated considering a mixing vessel discretized with a triangular grid. Future work will concern the development of realizable multivariate high-order convection schemes for moment transport, in order to reduce the numerical diffusion affecting the accuracy of the numerical predictions. The future inclusion of mass transfer terms such as boiling and condensation would be also be greatly beneficial for the nuclear industry as well.

2.2 References


CHAPTER 3. A SEMI-IMPLICIT SOLUTION ALGORITHM FOR POLYDISPERSE GRANULAR FLOWS

This chapter contains a draft of a manuscript in preparation to be submitted for publication.

3.1 Introduction

The ability to simulate gas-particle systems in which multiple classes of particles are present is essential in being able to accurately predict many different industrial applications and correctly understand how processes and results will be affected. Examples include biomass-sand reactors in which biomass reacts to form bio-oils and sand is used to enhance heat transfer (Ringer et al., 2006), fluidized beds with a distribution of particle sizes (Grace and Sun, 1991), and sediment transport in oil pipelines (Shirazi et al., 2015). The most common approach for large scale gas-particle flows is the Euler-Euler approach. This method uses the conditional mean of the conserved quantities (mass, momentum, and energy), a shared thermodynamic pressure, and for granular phases, one third the trace of the velocity covariance tensor, generally referred to as granular temperature or fluctuating granular energy. These equations are then closed using sub models for heat, mass, and momentum exchange, as well as kinetic theory closures for the particle phase quantities. While many methods for monodisperse (one particle diameter and density per computation cell) gas-particle flows have been studied (Passalacqua et al., 2011; van Wachem, 2000; Agrawal et al., 2001; Syamlal et al., 1993), methods for the simulation of polydisperse gas-particle flows in commercial codes have relatively specific purposes, without much room to generalize (for example, MFiX (Syamlal et al., 1993) allows for only one continuous phase). Other software has been developed, but due to the propriety nature of the codes Ahmad et al. (2013), the methods have not been documented. The primary difficulties in the simulation of polydisperse particulate flows is ensuring that the maximum particle volume fraction is not reached, ensuring that $\sum_k \alpha_k = 1$, and robustly handling the stiff
particle pressure term. Obeying these three conditions is very difficult because of the highly nonlinearity of the equations, all while conserving mass, momentum, and energy.

The derivations of kinetic theory transport equations were originally completed for only a single particle type (Chapman et al., 1990) and the most used instances of this neglect anisotropy in both the velocity distribution and particle stress tensor (Gidaspow, 1994). Several authors have completed derivations for the evolution of polydisperse granular systems with an isotropic particle stress tensor (Garzó et al., 2007; Zaichik et al., 2009; Huilin et al., 2001; Huilin and Gidaspow, 2003; Chao et al., 2011; Syamlal et al., 1993; Kong and Fox, 2019). Chao et al. (2011) also include an anisotropic particle stress. OpenFOAM currently used the numerical model of van Wachem (2000) which uses an isotropic model. The same formulation will be used to describe the granular temperature transport in this work as well.

Two different approaches can be used to help the stability of the gas-particle systems. These include adaptive time stepping, and additional coupling of the volume fraction transport equations and granular temperature transport. The first approach, that used in MFIX (Syamlal et al., 1993), is to solve for each of the granular phases using an adaptive time stepping method with local relaxation of the volume fraction to handle the stiff particle pressure term. Locally time stepping can lead to conservation issues (Passalacqua et al., 2011), and often the previous time step needs to be recovered if the solution becomes divergent. While preventing the simulation from crashing this does add additional computational cost, as well as numerical errors. In contrast, implicit solutions to the particle volume fraction transport allow for stable solutions, and mass conservation can be more easily enforced because the cells are all updated collectively.

The method developed will feature a semi-implicit method for the correction of the particle pressure flux, as well as the use of flux limiters to enforce packing limits and ensure mass conservation. The described method is applicable for m-continuous phases with n-particle phases. The work is developed in the OpenFOAM (OpenCFD Ltd., 2013a) framework, and is implemented the reactingEulerFoam solver. The equations presented will be for the incompressible, isothermal case, with one continuous phase. However, it is trivial to expand to m-continuous phases and the
reactingEulerFoam framework allows for additional physical models to be used (such as weakly compressible and anisothermal phase models).

Due to the lack of experiments that have been conducted to examine the dynamics of the polydisperse systems, only bidisperse cases will be presented. A verification of the general flow dynamics will be observed using a setting bed case in which the segregation of particle sizes due to drag will be examined, and a fluidized bed case using three particles sizes will show the segregation of sizes inside of the bed.

The remainder of this paper will be organized in the following way: Section 3.2 will describe the governing equations of polydisperse gas-particle flows with n-discrete particle phases. Section 3.3 will describe the discretization of the equation, and the limiting of particle fluxes. Section 4.5 details the full solution procedures for a multiphase system containing multiple particle type. Section 4.6 presents several test cases in order to validate the presented algorithm. Finally conclusion are presented in Section 3.6.

### 3.2 Governing Equations

The evolution of a collection of interacting phases can be described by the mass, momentum, and fluctuating granular energy (for particles) conservation equations of each phase (Drew, 1983; Chapman et al., 1990). The subscript pn will be used to donate the nth particle phase and the subscript g will denote the gas phase. The continuous gas phase is described by

\[
\frac{\partial}{\partial t} (\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g U_g) = 0,
\]

\[
3.1
\]

\[
\frac{\partial}{\partial t} (\alpha_g \rho_g U_g) + \nabla \cdot (\alpha_g \rho_g U_g \otimes U_g) = \nabla \cdot \tau_g - \alpha_g \nabla p + \sum_k K_{pk,g} (U_{pk} - U_g).
\]

\[
3.2
\]

The gas phase is considered to behave as a Newtonian fluid who’s stress tensor is defined as

\[
\tau_g = \alpha_g \rho_g \mu_g \left[ \nabla U_g + (\nabla U_g)^T - \frac{2}{3}(\nabla \cdot U_g)I \right].
\]

\[
3.3
\]
The gas and particle phases are coupled through the interfacial drag force, while the particle phases are coupled through drag as well as interactions in the transport of granular temperature. The drag between the gas phase and one particle phase is defined by Gidaspow (1994) by using the drag law of Wen and Yu (1966) when $\alpha_{pn} < 0.2$ and Ergun (Enwald et al., 1996) when $\alpha_{pn} > 0.2$.

$$K_{pn;g} = \begin{cases} \frac{3C_d \rho_g \alpha_{pn} \rho_p}{4d_{pn}} |U_g - U_{pn}| \alpha_g^{2.65} & \alpha_{pn} < 0.2 \\ 150 \mu_g \alpha_{pn}^2 + 1.75 \frac{\rho_g \alpha_{pn}}{\alpha_g d_{pn}} |U_g - U_{pn}| & \alpha_{pn} > 0.2 \end{cases}, \quad (3.4)$$

$$C_d = \begin{cases} \frac{24}{Re_{pn}} \left(1 + 0.15Re_p^{0.687}\right) & Re_{pn} < 1000 \\ 0.44 & Re_{pn} > 1000 \end{cases}, \quad (3.5)$$

$$Re_{pn} = \frac{\rho_g d_{pn} |U_g - U_{pn}|}{\mu_g}. \quad (3.6)$$

The time evolution equations for mass and momentum of the n-th particle phase are:

$$\frac{\partial}{\partial t}(\alpha_{pn} \rho_{pn}) + \nabla \cdot (\alpha_{pn} \rho_{pn} U_{pn}) = 0, \quad (3.7)$$

$$\frac{\partial}{\partial t}(\alpha_{pn} \rho_{pn} U_{pn}) + \nabla \cdot (\alpha_{pn} \rho_{pn} U_{pn} \otimes U_{pn}) = \nabla \cdot \tau_{pn} - \alpha_p \nabla p - \nabla (p_{pn} + p_{fr}) + \alpha_{pn} \rho_{pn} \mathbf{g}, \quad (3.8)$$

where $\alpha_{pn}$ is the n-th particle phase volume fraction, $\rho_{pn}$ the phase density, $U_{pn}$ the particle phase velocity vector, $\tau_{pn}$ the phase stress tensor, $p_{pn}$ and $p_{fr}$ are the nth particle-phase granular pressure and frictional pressure respectively, $U_g$ the gas-phase velocity vector, $\alpha_g$ the gas volume fraction, $p$ is the shared thermodynamic pressure, $\mathbf{g}$ the gravitational acceleration, $K_{pn;g}$ is the drag force due to the fluid drag on the n-th particle-phase, and $K_{pn;pj}$ is the particle-particle drag force between the n-th and j-th particle phases.
The particle phase viscous stress tensors, $\tau_{pn}$, are defined using the dynamic viscosity, $\mu_{pn}$, and bulk viscosity $\lambda_{pn}$, resulting in the non-Newtonian stress tensor defined as:

$$
\tau_{pn} = \rho_{pn} \mu_{pn} \left[ \nabla U_{pn} + (\nabla U_{pn})^T \right] + (\lambda_{pn} - \frac{2}{3} \mu_{pn}) (\nabla \cdot U_g) I.
$$  \hspace{1cm} (3.9)

$\theta_{pn}$ is used to denote the fluctuating particle energy, or more commonly known as the granular temperature. The particle phase viscosity includes the kinematic, collisional, and frictional contributions.

The particle-particle drag is defined by Syamlal (1987) and describes the momentum transfer between particle phase $n$ and particle phase $j$:

$$
K_{pn;pj} = \frac{3}{2} \left( 1 + e_{n,j} \right) \left( \frac{\pi}{2} + \frac{\pi^2}{8} \right) \alpha_{pn} \alpha_{pj} \rho_{pn} \rho_{pj} \left( d_{pn} + d_{pj} \right)^2 g_{0;n,j},
$$

where $e_{n,j}$ and $C_f_{n,j}$ are the coefficient of restitution and coefficient of friction between particle phase $n$ and particle phase $j$. The radial distribution function for particle phases $n$ and $j$ is defined as (Lebowitz, 1964)

$$
g_{0;n,j} = \frac{1}{\alpha_g} + \frac{3 d_{pn} d_{pj}}{\alpha_g^2 (d_{pn} + d_{pj})} \sum_k \alpha_{pk} \frac{d_{pk}}{d_{pk}},
$$

There is no particular form that is required for the drag term, therefore any drag model can be used, either for the gas-particle drag, or for the particle-particle drag.

The coefficients used in Eq. (3.12) are dependent on all granular temperatures, for example, the conductivity, $\kappa_{pn}$, dissipation due to collisions, $\gamma_{pn}$, and the production of granular energy due to drag, $J_{pn}$, etc. Additionally, the production of granular energy due to the gas-particle slip velocity, $J_{slip;pn}$ is also included (van Wachem, 2000). The full transport equation for the $n$-th particle phase can be seen below

$$
\frac{3}{2} \left[ \frac{\partial}{\partial t} (\alpha_{pn} \rho_{pn} \theta_{pn}) + \nabla \cdot (\alpha_{pn} \rho_{pn} \theta_{pn} U_{pn}) \right] =

(-p_{pn} I + \tau_{pn}) : \nabla U_{pn} + \nabla \cdot (\kappa_{pn} \nabla \theta_{pn}) +

-\gamma_{pn} + J_{pn} + J_{slip;pn},
$$

(3.12)
Because the solution algorithm only depends on the kinematic and frictional collision pressures, the other source terms will not be examined. Readers interested in the derivation or modeling can see Chapman et al. (1990); Huilin and Gidaspow (2003); Chao et al. (2011); Huilin et al. (2001); Syamlal et al. (1993). The Princeton models will be used for both granular pressure (Agrawal et al., 2001), and the frictional pressure models (Srivastava and Sundaresan, 2003). The granular pressure is defined as:

\[
p_{pn} = \alpha_{pn} \rho_{pn} \theta_{pn} \left[ 1 + 4 \sum_k (\eta_{n,j} \alpha_{pk} \theta_{n,k}) \right], \tag{3.13}
\]

where \(\eta_{n,j} = \frac{1 + e_{n,j}}{2}\). It is to be noted that the granular pressure must take the form of a coefficient times \(\theta_{pn}\) in order to treat the granular pressure implicitly resulting in an isotropic assumption on the particle stress due to a small Knudsen number. The frictional pressure is defined as

\[
p_{fr} = \begin{cases} 
10^{24} \left( \alpha_p - \alpha_{p,min}^* \right)^{10} & \alpha_p < \alpha_{p,min}^* \\
Fr \frac{\left( \alpha_p - \alpha_{p,min}^* \right)^r}{\left( \alpha_{p,max} - \alpha_p \right)^p} & \alpha_{p,max} > \alpha_p > \alpha_{p,min}^* \\
0 & \alpha_p < \alpha_{p,min} 
\end{cases} \tag{3.14}
\]

\(\alpha_p\) is the sum of all particle phases, \(\alpha_{p,min}^*\) is the minimum particle volume fraction at which frictional stress becomes active, and \(\alpha_{p,fr,min}\) is the minimum volume fraction at which the frictional model switches to using a power low. The latter is generally set close to the packing limit for the presented model. Because the packing limit can vary spatially depending on the concentration of particles of different size, a minimum ratio, \(r_{fr,min}\), is instead used where \(\alpha_{p,fr,min} = r_{fr,min} \alpha_{p,max}\).

The typical values of the coefficient used in the frictional model are \(Fr = 0.05\), \(p = 5\), \(r = 2\), and \(\alpha_{p,min}^* = 0.5\). Because the frictional model is only a function of the total particle phase volume fraction, the frictional pressure force is applied to all particle phases based on the phase solid volume fraction relative to the total solid volume fraction (i.e. scaled by \(\alpha_{pn}/\alpha_p\)). The frictional component of viscosity is also described by Srivastava and Sundaresan (2003) and includes the total particle velocity and volume fraction.
3.3 Discretized equations

The solution of the mass transport of the particle-phases adds increased challenges in comparison to the two fluid phases due to complication of transport coefficients, as well as the total solid-phase packing limit which can vary in space, and limits the local particle fluxes. In addition, the packing limit of the individually phases must also be respected. The conservation of mass within all phases must also occur at the same time in addition to conservation of total mass which is ensured by a divergence-free volume-fraction-weighted velocity. The solution to these problem will be presented in the following order; first the discretized momentum equations will be presented; next the semi-implicit solution to the volume fraction transport will be described; finally, the flux limiting methods will be presented.

3.3.1 Discretized momentum equations

The gas and particle phase are written in their semi-discrete form as

\[ A_{pn} U_{pn} = \mathbb{H}_{pn} - \alpha_{pn} \nabla p - \nabla (p_{pn} + p_{fr}) + \alpha_{pn} \rho_{pn} g + K_{pn;g} (U_{g} - U_{pn}) + \sum_{j} K_{pn;j} (U_{pj} - U_{pn}), \]

(3.15)

and

\[ A_{g} U_{g} = \mathbb{H}_{g} - \alpha_{g} \nabla p + \alpha_{g} \rho_{g} g + \sum_{j} K_{pj;g} (U_{pj} - U_{g}), \]

(3.16)

where \( A \) and \( \mathbb{H} \) are defined in terms of the linear operator matrix, \( A^f \), that is built from the phase momentum equations, with the following definitions

\[ A_i = \text{diag}(A^f_i), \]

(3.17)

\[ \mathbb{H}_i = A^s_i - A^\text{off}_i U^\text{old}_i. \]

(3.18)

\( A_i \) is defined as the diagonal coefficients of the full matrix, \( A^\text{off}_i = A^f_i - A_i \) is the off diagonal matrix, and \( A^s \) are the source terms of the equations. \( U^\text{old}_i \) is defined as the velocity at the beginning
of the prediction step. The unsteady, transport, stress, and remaining source terms are all included in the matrix $A_f$. Using the identities,

$$\lambda_{pn} = \frac{1}{A_{pn} + K_{pn;g} + \sum_k K_{pn;pk}}, \quad (3.19)$$

and

$$\lambda_g = \frac{1}{A_g + \sum_k K_{pn;g}}, \quad (3.20)$$

This results in an estimate of the phase velocities which will later be corrected using the pressure gradient,

$$U_{pn} = \lambda_{pn} H_{pn} - \lambda_{pn} (\alpha_{pn} \nabla p + \nabla (p_{pn} + p_{fr})) + \lambda_{pn} \alpha_{pn} \rho_{pn} g + \lambda_{pn} (K_{pn;g} U_{g} + \sum_k K_{pn;pk} U_{pk}), \quad (3.21)$$

and

$$U_g = \lambda_g H_{g} - \lambda_g \alpha_g \nabla p + \lambda_g \alpha_g \rho_g g + \lambda_g \sum_k K_{pk;g} U_{pk} \quad (3.22)$$

details the optional step of re-substitution to eliminate the other phase velocities from the n-th phase in the semi-discrete equation by means of inverting a coefficient matrix. This step will not be used the presented cases.

### 3.3.2 Pressure equation and fluxes

The pressure equation is derived using the constraint that the divergence of the total flux, $\nabla \cdot (\sum_i \alpha_i U_i)$, is equal to zero. The phase-flux, $\phi_i$, is found by interpolating the cell centered values of the phase velocities, denoted by the subscript $f$, and dotting with the surface normal vector, $S$ (where the magnitude is the surface area of the face). This leads to

$$\phi_{pn} = \lambda_{pn;f} (H_{pn} + \alpha_{pn} \rho_{pn} g) \cdot S - \lambda_{pn;f} \alpha_{pn;f} |S| \nabla \perp p$$

$$+ \lambda_{pn;f} \left( K_{pn;g;f} \phi_g + \sum_k K_{pn;pk;f} \phi_{pk} \right) \quad (3.23)$$

$$- \lambda_{pn;f} G(\alpha_{pn;f}) |S| \nabla \perp \alpha_{pn},$$
and
\[ \phi_g = \lambda_{g,f} (\mathbb{H}_g + \alpha_g \rho_g g)_f \cdot \mathbf{S} + \lambda_{g,f} \sum_k K_{pk;g;f} \phi_{pk} - \lambda_{g,f} \alpha_{g,f} |\mathbf{S}| \nabla \cdot \mathbf{p}, \] (3.24)

where \( G(\alpha_{pn}) \) is defined as the derivative of the particle pressure (combination of frictional and granular) with respect to \( \alpha_{pn} \), i.e.
\[ G(\alpha_{pn}) = \frac{\partial (p_{pn} + p_{fr})}{\partial \alpha_{pn}}, \] (3.25)

and \( \nabla (p_{pn} + p_{fr}) = G(\alpha_{pn}) \nabla \alpha_{pn} \). While \( G(\alpha_{pn}) \) includes contributions from all of the particle phases, only the derivative with respect to the n-th phase is taken.

Volumetric conservation is enforced using
\[ \nabla \cdot \phi = \nabla \cdot (\alpha_g \phi_g) + \sum_k \nabla \cdot (\alpha_{pk} \phi_{pk}) = 0, \] (3.26)

which results in
\[ \nabla \cdot \phi^0 = \nabla \cdot \left[ \left( \lambda_g \alpha_g + \sum_k \lambda_{pn\alpha_{pn}} \right) |\mathbf{S}| \nabla \cdot \mathbf{p} \right], \] (3.27)

where \( \phi^0 \) is the flux in which the pressure gradient contribution has been removed. Finally, we obtain the estimation of the phase flux prior to the pressure correction
\[ \phi_{pn}^0 = \lambda_{pn;f} (\mathbb{H}_{pn} + \alpha_{pn} \rho_{pn} g)_f \cdot \mathbf{S} - \lambda_{pn;f} G(\alpha_{pn;f}) |\mathbf{S}| \nabla \cdot \mathbf{p}, \] (3.28)

and
\[ \phi_g^0 = \lambda_{g;f} (\mathbb{H}_g + \alpha_g \rho_g g)_f \cdot \mathbf{S} + \lambda_{g;f} \sum_k K_{pk;g;f} \phi_{pk}, \] (3.29)

After solving Eq. (3.27), the fluxes are corrected using
\[ \phi_{pn} = \phi_{pn}^0 - \lambda_{pn;f} \alpha_{pn;f} |\mathbf{S}| \nabla \cdot \mathbf{p}, \] (3.30)

and
\[ \phi_g = \phi_g^0 - \lambda_{g;f} \alpha_{g;f} |\mathbf{S}| \nabla \cdot \mathbf{p}. \] (3.31)
3.3.3 Continuity equations

Unlike the typical approach taken in the monodisperse, two-fluid case, where only one continuity
equation needs to be solved and the other volume fraction can be found using the relation $\alpha_g + \alpha_p = 1$, the multi-fluid model requires that all continuity equations are solved. This can lead to numerical errors that cause the sum of volume fractions to no longer exactly equal one, resulting in poor mass conservation. Listed below are the conditions that must be satisfied upon solving Eq. (3.7) and (3.1):

1. $\nabla \cdot \left( \alpha_g \phi_g + \sum_j \alpha_p \phi_p \right) = \nabla \cdot \phi = 0$
2. The individual volume fraction can not be greater than the monodisperse packing limit, $\alpha_{pn} < \alpha_{pn,max}$
3. The total particle volume fraction can not be greater than the total packing limit, $\sum_j \alpha_p j < \alpha_{p,max}$
4. $\alpha_g + \sum_k \alpha_p k = 1$.

These criteria are enforced using the following methods: Condition 1 is enforced by limiting
the fluxes so that the sum of the fluxes in a cell is 0, conditions 2 and 3 are enforced using the
fluxing limiting scheme MULES (Weller, 2006) along with the semi-implicit treatment of the particle
pressure (both expanded on further below). If condition 1 is enforced, then the total volume fraction
is not changing in time so condition 4 is also satisfied.

3.3.3.1 Removal of particle pressure flux

The continuity equation for the n-th particle phase is given by

$$\frac{\partial \alpha_{pn}}{\partial t} + \nabla \cdot \left( \alpha_{p,n} \phi_{pn} \right) = 0.$$  (3.32)

Using the approach taken by Weller (2006) and Passalacqua et al. (2011), the n-th particle flux
is written in terms of the conservative total flux, $\phi$, and the combination of the relative fluxes, $\phi_{r,i,m}$
where \( m \) and \( i \) includes all particle phases as well as the gas phase. Using

\[
\phi = \sum_i \alpha_i \phi_i, \quad (3.33)
\]

\[
\phi_{r;i,m} = \phi_i - \phi_m. \quad (3.34)
\]

The individual phase fluxes are written in terms of the total and relative fluxes is

\[
\phi_i = \phi + \sum_{m;i \neq m} \alpha_m \phi_{r;i,m}. \quad (3.35)
\]

No special treatment is needed for the gas phase, but due to the stiffness of the particle pressure flux, removing the particle pressure and re-adding it implicitly has been shown to improve stability (Passalacqua et al., 2011).

Using the above definitions and subtracting the particle pressure, the following equation is solved for the given particle volume fractions,

\[
\frac{\partial \alpha_{pn}}{\partial t} + \nabla \cdot \left[ \alpha_{pn;f} \left( \phi_i^* + \sum_i \alpha_{i;f} \phi_{r;i,m}^* \right) \right] - \nabla \cdot \left[ \alpha_{pn;f} (1 - \alpha_{pn;f}) \left( \frac{\lambda_{pn} G(\alpha_{pn})}{\rho_{pn}} \right)_f |\mathbf{S}| \nabla \perp \alpha_{pn} \right] = 0, \quad (3.36)
\]

where the superscript * denotes a flux with the particle pressure contribution removed. In order for \( \sum \alpha_i = 1 \) to be enforced the fluxes must be held constant after the final limiting of the fluxes to ensure that the total flux is divergence free. If the particle volume fractions are implicitly updated after, like what is typically done for two-phase simulations, the difference between the removed particle pressure flux and the flux given from the linear system (Eq. (3.36)) is not consistent, and leads to non-negligible mass conservation errors. To remedy this, Eq. (3.36) is used to correct the particle pressure flux which is then held constant throughout the advection procedure. This is done by neglecting \( \phi_i^* \), leading to an unsteady diffusion equation that is solved and produces a correction term to the particle flux. This correction is then subtracted from the particle pressure flux at each flux limiting step (MULES).
3.3.3.2 Flux limiting

After the particle pressure fluxes are corrected, the volume fractions are advanced in time using the explicit MULES advection procedure in which the phase fluxes use the form seen in Eq. (3.35). The volumetric fluxes \((\alpha_k f \phi_k)\) are limited to ensure that the maximum phase volume fraction limit is not reached, and are then explicitly updated using the limited flux. Once the individual phases have been limited, all particle phases volume fraction and fluxes are summed using \(\alpha_p f \phi_p = \sum_k \alpha_k f \phi_k\). This flux is limited using the same procedure as the individual phases, but the limiting coefficients that are calculated for the combination of particle fluxes are then applied to the individual particle phase fluxes. Lastly, \(\nabla \cdot \phi = 0\) is enforced by limiting the remaining continuous phase fluxes so the total flux is divergence free. This is done by scaling the residual flux by the relative volume fraction of the continuous phases. Only the volume fraction flux \((\alpha_k f \phi_k)\) is limited, and not the actual phase flux \((\phi_k)\) so that momentum is still conserved when the pressure equation is solved (OpenCFD Ltd., 2013b).

3.4 Solution procedure

The solution procedure has been implemented in reactingMultiphaseEulerFoam which is designed to handle anisothermal, weakly compressible flows, but to simplify the procedure, the isothermal and incompressible case is described. A similar procedure can be found in Passalacqua et al. (2011), and is as follows:

1. The granular temperature transport equations are solved for all particle phases.

2. Calculate \(G(\alpha_{pn})\) at the cell centers and interpolate to the cell faces.

3. Begin iterations on the volume fractions

   (a) Implicitly update the particle pressure flux using Eq. (3.36).

   (b) Added change in total particle pressure flux to continuous phase volume fraction flux

   (c) Begin sub-time steps for explicit volume fraction transport.
i. Limit the individual volume faction to their individual maximums

ii. Sum the granular phases and find the limiting coefficients to ensure the total particle volume fraction is less than the particle packing limit, and scale individual fluxes

iii. Limit the continuous phase fluxes so that the total flux is divergence free

(d) If the convergence criteria is not met, return to step (a).

4. Update momentum transfer coefficient using the new volume fractions.

5. Construct the phases momentum equations, excluding the thermodynamic pressure terms.

6. Begin the pressure correction loop.

   (a) Estimate the phase velocities using $\frac{H_k}{A_k}$.

   (b) Calculate the total flux using the predicted phase fluxes, where the pressure gradient has been removed.

   (c) Start non-orthogonal correction loop

      i. Construct the pressure equation.

      ii. Solve the pressure equation.

   (d) Correct the phases fluxes using the new pressure gradient

   (e) Update the phase velocities either using a flux reconstruction of the definition in Eq. (3.15) and (3.16).

   (f) If the convergence criteria is not met return to step 6.

7. Advance to the next time step.

3.5 Validation results

One verification and two validation cases will be presented using bidisperse distributions. First the dynamics of a settling bed is examined. Next the segregation of sizes in a fluidized bed is compared to Ahmad et al. (2013). Finally a cyclic, vertical riser is compared to the results of Chao et al. (2011); Mathiesen et al. (2000).
3.5.1 Settling Suspension

The first case used to validate the solver will the time evolution of an initially uniform suspension of bi-disperse particles that settles. This case will be used to show the segregation that occurs to the difference in particle sizes. The column has dimensions of 0.15 m x 1 m, and was discretized in to 30 x 200 computational cells. Initially both particle sizes have a uniform volume fraction of 0.15, or a total particle volume fraction of 0.3. The the smaller particle phase has a diameter of 100 $\mu$m, and the larger has a diameter of 600 $\mu$m, and both have densities of 2500 kg/m$^3$. The particles are initially at rest when they are released and allowed to fall.

Fig. 3.1 shows the volume fractions of the two different particle sizes at four different points in time. It can be seen that the larger particles fall faster than the small particles and accumulate...
Figure 3.2  Plots of the volume averaged particle diameter versus height once the suspension has settled.

Figure 3.3  Particle vertical velocities at $y = 0.2$ m.

Figure 3.4  Particle vertical velocities at $y = 0.5$ m.
faster at the bottom of the column. This corresponds to the expected behavior of the system since the stokes number of the smaller particles is less than that of the larger particles, resulting in more resistance due to the slower moving fluid. This can be seen in Fig. 3.2 where the average diameter becomes small at the top of the particle phases, and larger at the bottom. Additionally, the velocities of the two particle phases are shown in Fig. 3.3 and 3.4, and again show the higher downward velocity of the larger particles.

### 3.5.2 Bidisperse fluidized bed

Next, results are compared to that of both experimental and an existing polydisperse granular solver (Ahmad et al., 2013). Two particle sizes of 120 µm and 185 µm, both with equal volume fractions, are initially at rest. The bed is the fluidized with an inlet air velocity of 0.1 m/s. The computation domain is 1 m high by 0.12 m wide and is discretized in to 280 x 60 computational cells with higher wall resolution. The average volume fraction of the larger particles in six different regions is then averaged of the region volume. The instantaneous profiles of the total particle volume fraction, as well as the individual size are shown in Fig. 3.5. The average total volume fraction versus height is shown in Fig. 3.6.

The segregation of particle sizes is seen to be strongest at the bottom of the bed. This can be seen in the plot versus height, and as a result the average total particle volume fraction is lower in the segregated region due to the lower packing fraction of monodisperse mixture. The main difference between volume fraction profiles of the presented solver and the results of Fluent is likely due to the frictional model used. The Princeton model was used for the presented work while fluent used that of Schaeffer. This leads to stronger segregation due to the stronger influence of drag on the hydrodynamics of the particles phases.

### 3.5.3 Bidisperse vertical riser

The final case is that of a cyclic vertical riser and is compared to the experimental results of Mathiesen et al. (2000) and the computational results of Chao et al. (2011). Two particle sizes
Figure 3.5  Instantaneous solid volume fractions at $t = 30.0$ s.

Figure 3.6  Average distribution of larger particle versus bed height.
of 120 µm and 185 µm, both with equal volume fractions. A cyclic computational domain of 0.3 m high by 0.032 m in width is used. The average air velocity in the riser is kept at a constant velocity or 1 m/s using a mean pressure gradient forcing. The average total volume fraction, as well as the small \((s_1)\) and large \((s_2)\) volume fractions are shown plotted against the results of Chao et al. (2011) and the experiments of Mathiesen et al. (2000). The time averaged profiles of the total particle volume fraction can be seen in Fig. 3.7, as well as the individual size are shown in Fig. 3.8, and the standard deviation of the particle velocity in Fig. 3.9 \((\sqrt{3(\theta_{p1} + \theta_{p2})})\). The simulation was run for a total of 50 s and averaged for 45 s.

The results of the total volume fraction as well as the small particle volume fraction match fairly well between the results of Chao et al. (2011) and OpenFOAM, however the prior appear much more parabolic in profile, in comparison to a flat profile in the center of the riser seen in both the current method and that of Mathiesen et al. (2000). The difference in the larger particle volume fraction profile is likely due to the fact that the large particle in the case presented were allowed to fall back through the top, so the segregation of sizes was not as strong. Additionally, the standard deviation of velocity Shows that granular energy is highest at the wall. This is due to the fact that
Figure 3.8  Average solid volume fractions.
granular energy is produced at the center of the riser due to drag and is then transported towards the walls. Because the particles are nearly elastic, only a small amount of energy is dissipated, and is built up at the walls.

3.6 Conclusions

A new solution algorithm for the simulation of polydisperse granular flows has been presented in the Eulerian, multi-fluid frame work. The algorithm uses flux limiters and a semi-implicit corrector for the particle pressure flux to ensure solution stability and accuracy. The presented algorithm has been validated using a settling bidisperse bed where the results qualitatively match the expected results. The results show that the larger particles fall faster, and therefore due to the differences in the drag force on different particle sizes, there is a higher concentration at the bottom of the bed. Using a fluidized bed, it was also shown that the fluidization of a particle bed with a distribution of sizes will begin to segregate, and on average a similar result to the settling bed is seen, where larger particles tend to settle at the bottom of the bed while smaller particles drift towards the top of the bed. The segregation profile of the bed also compares well to that of Fluent as well as experimental results. Finally, the average profiles of the volume fractions and granular temperatures has been shown to match both experimental data as well as previous simulation results. Because of the fact that the solution method has been implemented in OpenFOAM’s reactingEulerFOAM framework,
this also allows for the addition of additional physics to be included, such as reactions, species transport, population balance modeling, and mass transfer. This results in a solution procedure that is general, and can be used for a wide range of cases ranging from simple geometries, to completely unstructured meshes.

3.7 References


CHAPTER 4. A QUADRATURE-BASED MOMENT METHOD FOR THE EVOLUTION OF THE JOINT SIZE VELOCITY NUMBER DENSITY FUNCTION OF A PARTICLE POPULATION

This chapter contains a draft of a manuscript in preparation to be submitted for publication.

4.1 Introduction

The approximate solution of kinetic equations describing the spatio-temporal evolution of a particle population has a wide range of applications, from non-equilibrium flows and rarefied gases to multiphase disperse flows. In case the population of particles under consideration involves particles of different sizes, which can evolve due to phenomena such as aggregation, breakage, and growth, the distribution characterizing the particle population is a joint size-velocity number density function. Some of these particles may not follow the fluid streamlines due to a non-negligible inertia, leading to the phenomena of particle trajectory crossing (Desjardins et al., 2008). The assumptions regarding the velocity distribution of a population of particles fall into three categories. First, the zero Stokes number case in which particles immediately respond to changes in the velocity flow field. The second is that in which the Stokes number is small, but not zero, creating a situation where particles of a given size, locally move at the same velocity, with particles characterized by different sizes have different velocities. This case can be modeled under the monokinetic assumption (Massot, 2007) by only knowing the mean velocity conditioned on size. The last case is that in which the particles have a significant inertial (St >> 1). In this case, in the dense limit the VDF tends towards the Maxwellian, and in the dilute case, it indicates non-equilibrium. In this case, it is then required to consider higher-order moments of the VDF to satisfactorily describe the physics of the flow. A review of methods for these three ranges of Stokes number are presented below.
The evolution of a particle population with negligible inertia was originally studied by Randolph (1964). Several methods have been used to solve for this evolution, such as the method of classes (Ramkrishna, 2000) and the method of moments, of which the quadrature based method of moments is a well-known example (McGraw, 1997; Marchisio and Fox, 2013). Both of these methods have been developed to numerically solve this evolution equation. The assumption of zero Stokes number is acceptable when describing the evolution of either very dilute particle suspensions or particles with a very small size as in flash nano-precipitation (Cheng et al., 2010) and soot formation (Zucca et al., 2006) processes.

The second case of a mono-kinetic dispersed phase is often employed in the description for either low density materials such as dispersed phase bubbles, or small particles and droplets. These systems have been discussed in literature using different formulations of the method of classes (Laurent and Massot, 2001; Frank et al., 2005; Bannari et al., 2008), or QBMM in which the size-velocity moments are used to approximate the underlying distribution (Fox et al., 2008; Massot et al., 2010; Yuan and Fox, 2011; Heylmun et al., 2019). The first two methods using QBMM have been developed using the direct quadrature method of moments (DQMOM) for sprays, while the second two use an adaptive inversion procedure to evolve the moments of a joint size-velocity distribution of a population of bubbles.

The final case of particles with a Stokes number much greater than one is typical of gas-particle flows. Such flows can be described either with Lagrangian methods (Riley, 1974; Capecelatro and Desjardins, 2013), or in a continuum framework, by the kinetic theory of granular flows (KTGF) (Chapman et al., 1990; Gidaspow, 1994). Several formulations of KTGF exist ranging from that used to derive models in the collisional limit which particle properties are transported and changed due to collisions (Kn ∞ 1) leading the velocity distribution to be Maxwellian, to methods specifically developed for to describe cases where collisions are not be the principal method of property transport and evolution, such as in inviscid or dilute particulate flows. Derivations of the prior have primarily been for monodisperse particle populations or fixed sizes. Generally these derivations assume an isotropic velocity distribution function (VDF) where mean velocity and granular
temperatures (velocity variance) completely describe the particle VDF. There have also been extensions to this where a polydisperse system of particles in evolved in space and time (Huilin et al., 2001; Garzó et al., 2007; Chao et al., 2011) but neglect the evolution of the size distribution. Kong and Fox (2019) has included the evolution of the particle size distribution using the quadrature methods to approximate the distribution. More recent methods such as Passalacqua and Fox (2011) have included the transport of higher order moments to more accurately represent the VDF, but still neglect changes in the size distribution. While these methods allow for improved predictions compared to the commonly used two-fluid description, in which both phases obey the Navier-Stokes equations (Drew, 1983), they also leave room for improvement, especially in regards to anisotropy of the velocity distribution and a more complete description of the size evolution of particles.

Methods for describing the joint size-velocity distribution and its coupling to a fluid phase have been described in theory using moment methods (Marchisio and Fox, 2013; Yuan and Fox, 2011), but these methods have not been implemented in a manner that allow for a simulation of this full distribution to be evolved in space and time. For this reason, this work will focus on the numerical aspects of a robust approach, using the quadrature based method of moments, to approximate the discrete distribution using the moments of the size-velocity distribution. This produces a set of discrete weights, size, and velocity abscissae which are used to numerically integrate terms in the moment transport equations, and calculate the source terms required to evolve the full distribution. The goal of this method is to obtain a stable numerical method that can be applied to any number of dispersed multiphase flow problems.

The remaining sections will be organized in the following manner: in Section 4.2 the moment transport equations derived from the generalized population balance equation are presented. Section 4.3 describes the quadrature-based method of moments and the inversion procedure used to obtain an approximate NDF from the transported moments. The closures to both advection and source terms are derived, and their approximations are presented in Section 4.4. Section 4.5 describes the numerical procedure for the full solution to the moment transport equations. Finally in Section 4.6, 0-D, 1-D, and 2-D test cases with 2 and 3 dimensional velocity distribution test cases
are presented to show the capabilities as well as the robustness of the moment inversion algorithm and solution procedure.

4.2 Governing Equations

We begin by introducing the generalized population balance equation (GBPE) used to describe the evolution of the joint size-velocity number density function (NDF) that characterizes a polydisperse particulate system. The generalized population balance equation can be seen in Eq. (4.1), where \( f = f(t, x, \xi, v) \) is the number density function, and is dependent on time, \( t \), position, \( x \), particle size, \( \xi \), and particle velocity \( v \).

\[
\frac{\partial f}{\partial t} + \nabla_x \cdot (fv) + \nabla_\xi [G(\xi)f] + \nabla_v \cdot \{[A(\xi, v) + g]f\} = C. 
\]

(4.1)

\( \nabla_x \cdot (fv) \) represents the advection of the NDF in physical space, \( \nabla_\xi \cdot [G(\xi)f] \) is the advection term with respect to \( \xi \) and represents growth, \( \nabla_v \cdot \{[A(\xi, v) + g]f\} \) represents the change in the velocity components of the NDF due to external accelerations such as drag \( (A) \), and the gravitational acceleration \( g \). It should be noted that \( A \) can be dependent on both size and velocity, but it will not change the distribution of particles sizes. Lastly, \( C \) accounts for source terms that may change both the size and velocity components such as aggregation, breakup, and collisions which only affect the velocity.

While methods for accurately solving Eq. (4.1) directly do exist, they are computationally expensive for engineering applications involving systems with a large number of particles (Fox et al., 2008). In several cases, however, a detailed knowledge of the NDF is not necessary and the accurate knowledge of some of its moments is sufficient. In these situations, the adoption of moment methods allows an approximate solution to Eq. (4.1) to be found at a significantly lower computational cost. In these methods, the statistical moments of the NDF are defined as:

\[
M_{pijk} = \int_{\mathbb{R}^+} \int_{\mathbb{R}^3} \xi^p v_x^i v_y^j v_z^k f(t, x, \xi, v) dv d\xi, 
\]

(4.2)

where \( M_{0000} = \varepsilon_p \) is the volume fraction, \( M_{1000} = \varepsilon_p d_p \) the volume weighted average particle diameter, and \( \langle M_{0100}, M_{0010}, M_{0001} \rangle = \varepsilon_p u_p \) the volume weighted average velocity. The choice of
the moment scaling so that \( M_{0000} \) is the volume fraction rather than the number density is made to avoid numerical difficulties caused by the very large number of particles typically encountered in applications. For the same reason, the particle diameter is considered instead of the particle volume or mass.

The moment transport equations are derived by multiplying the generalized kinetic equation by the necessary variables, i.e. \( \xi^p, v^i_x, v^j_y, \) and \( v^k_z, \) and integrating over the entire space of internal coordinates (\( \Omega = \mathbb{R}^+ \times \mathbb{R}^3 \)) leading to:

\[
\frac{\partial M_{pijk}}{\partial t} + \nabla \cdot F_{pijk} + \int_{\mathbb{R}^+} \int_{\mathbb{R}^3} \xi^p v^i_x v^j_y v^k_z f(t, x, \xi, v) [A(v) + g] \, dv \, d\xi = C_{pijk} \tag{4.3}
\]

which is the transport equation for moment \( M_{pijk}, \) where the moment flux \( F_{pijk} \) is defined as \( <M_{p,i+1,j,k}, M_{p,i,j+1,k}, M_{p,i,j,k+1}>. \) All the terms on the right-hand side of Eq. (4.3) are unclosed because they depend on \( f. \) Closures need then to be provided for the flux term \( F_{pijk}, \) the acceleration \( A(v), \) and the term \( C_{pijk}. \) One effective approach to formulate these closures is represented by the quadrature method of moments (McGraw, 1997; Fox, 2003; Marchisio and Fox, 2013). This approach is further developed in this work to address problems involving joint size-velocity distributions.

### 4.3 The quadrature method of moments

In order to close advection and source terms of Eq. (4.3), the size-velocity NDF is reconstructed using the quadrature method of moments (QBMM) (Marchisio and Fox, 2013). The number density function, \( f(\xi, v, x, t) \) is approximated using a summation of \( N \) Dirac delta distributions

\[
f(\xi, v) \approx \sum_{\alpha} w_{\alpha} \delta(\xi - \xi_{\alpha}) \delta(v - v_{\alpha}), \tag{4.4}
\]

where \( N \) is set to achieve the required order of accuracy for the distribution, \( w_{\alpha} \) are the quadrature weights, \( \xi_{\alpha} \) the size abscissae, and \( v_{\alpha} \) the velocity abscissae. Using this approximation, the moments of the distribution can be expressed in terms of weights and abscissae as

\[
M_{pijk} = \sum_{\alpha=1}^{N_{\xi}} \sum_{\beta_x=1}^{N_{vx}} \sum_{\beta_y=1}^{N_{vy}} \sum_{\beta_z=1}^{N_{vz}} w_{\alpha,\beta_x,\beta_y,\beta_z} \xi^p_{\alpha,\beta_x,\beta_y,\beta_z} v^i_x v^j_y v^k_z, \tag{4.5}
\]
where $w_{\alpha,\beta_x,\beta_y,\beta_z}$ are the integrated conditional weights of the distribution, and $v_x, v_y,$ and $v_z$ are the conditional velocity abscissae. The quadrature method of moments uses this approximate distribution to close source terms and compute additional higher order moments required for the advection term of the velocity moments. The form of Eq. (4.5) is that of a linear combination of Vandermonde systems which will be used to define the conditional quadrature method of moments procedure in the following section.

4.3.1 Moment inversion algorithm

The proposed procedure to compute the quadrature weights and abscissae is based on the idea of computing conditional moments using the quadrature in the directions inverted prior, and the true moments required to solve the linear system (Eq. (4.6)). The proposed algorithm is a variant of CQMOM presented by Yuan and Fox (2011), and uses the size direction as the primary direction (no conditioning), and leverages the efficiency and robustness of the velocity moment inversion procedure introduced in Fox et al. (2018). It should be noted that although the algorithm of Fox et al. (2018) is used to invert the conditional velocity moments in this work, it is not a requirement allowing other velocity moment inversion algorithms to be used. For example, the extended 23-moment inversion procedure outlines in the appendix of Fox et al. (2018) or the monokinetic inversion (Yuan et al., 2014).

The first step in inverting the given four-dimensional moment set is to compute the $N_{\xi}$ size-conditioned velocity moment sets. This is done by first inverting the pure size moments, i.e. $M_{000}$. From this, the size weights and abscissae, $w_{\alpha}$ and $\xi_{\alpha}$, are found using the Wheeler algorithm (Wheeler, 1974). Next, the conditional moments of the velocity distribution are found using the linear systems

$$
[V][R] = \begin{bmatrix} v_{0,\xi} \\ v_{1,\xi} \\ \vdots \\ v_{N_{\xi}-1,\xi} \end{bmatrix} = \begin{bmatrix} M_{0,\xi} \\ M_{1,\xi} \\ \vdots \\ M_{N_{\xi}-1,\xi} \end{bmatrix},
$$

(4.6)
where \( q \) are the indexes of the required moments in the CHyQMOM inversion (i.e. \((0, 0, 0), (1, 0, 0), (2, 0, 0), (3, 0, 0), (4, 0, 0), (0, 1, 0), (1, 1, 0), (0, 2, 0), (0, 3, 0), (0, 4, 0), (0, 0, 1), (1, 0, 1), (0, 1, 1), (0, 0, 2), (0, 0, 3)\) and \((0, 0, 4)\)), \( \nu \) are the moments of the size conditioned velocity distribution, \( M \) are the moments about the origin of the full distribution, \([V]\) a Vandermonde matrix, and \([R]\) are defined as

\[
[V] = \begin{bmatrix}
1 & 1 & \cdots & 1 \\
\xi_0 & \xi_1 & \cdots & \xi_{N_\xi} \\
\vdots & \vdots & \ddots & \vdots \\
\xi_0^{N_\xi-1} & \xi_1^{N_\xi-1} & \cdots & \xi_{N_\xi}^{N_\xi-1}
\end{bmatrix}, \tag{4.7}
\]

\[
[R] = \begin{bmatrix}
w_0 \\
w_1 \\
\vdots \\
w_{N_\xi-1}
\end{bmatrix}. \tag{4.8}
\]

Finally we solve

\[
\begin{bmatrix}
\nu_{0, q} \\
\nu_{1, q} \\
\vdots \\
\nu_{N_\xi-1, q}
\end{bmatrix} = [R]^{-1}[V]^{-1}\begin{bmatrix}
M_{0, q} \\
M_{1, q} \\
\vdots \\
M_{N_\xi-1, q}
\end{bmatrix}, \tag{4.9}
\]

to obtain the moments of the velocity distribution conditioned on the size \( \xi_\alpha, \nu_\alpha, q \). The \( N_\xi \) size-conditioned velocity moment sets are inverted using the CHyQMOM inversion procedure described in Fox et al. (2018). This produces the conditional weights \( w_{\alpha, \beta_x, \beta_y, \beta_z} \) which are scaled by the size weight \( w_\alpha \) so that they can be used in the form seen in Eq. (4.5), as well as the conditional velocity abscissae, \( v_{\xi; \alpha, \beta_x}, v_{\nu; \alpha, \beta_y}, \) and \( v_{\rho; \alpha, \beta_x, \beta_y, \beta_z} \). The approximation of the entire four-dimensional size-velocity distribution now allows for the numerical integration of both source terms and advection.
4.4 Closures to the moment transport equations

We detail in this section the closures, based on the quadrature definition in Section 4.3, for the advection and source terms.

4.4.1 Advection

One of the most important step in formulation of a stable solution procedure to solve the moment transport equations is the calculation of the moment advection terms. The difficulty in moment advection is two-fold when the NDF consist of internal velocity components. First, the standard moment transport problem of ensuring moment set realizability is present, however less strict for velocity moments since the velocity distribution in supported on $\mathbb{R}^3$. The size moments are restricted to $\mathbb{R}^+$ though, leading to more restrictive conditions to ensure the realizability of the moment set. This is due to the fact that standard interpolation schemes of order higher than one can result in an unrealizable moment set due to the fact that the use of multiple limiters on the multiple moments do not guarantee the resulting set of limited moments is realizable (Wright, 2007). The second complication comes about because, unlike simple, non-inertial particle transport which is advected with only a mean velocity, each discrete particle size is transported with its own, unique velocity distribution. This means that the flux contribution for each moment must be calculated per each size distribution, then summed to obtain the total moment flux. The numerical integration of the moment fluxes will be calculated using kinetic based fluxes (Yuan and Fox, 2011). This allows for both first order and quasi-second order schemes to be used. Both use a flux reconstruction method according to which

$$F_{p,i,j,k} = \sum_{\alpha}^{N} \left( w_{\alpha} \xi_{p,\alpha}^{i} v_{x,\alpha}^{j} v_{y,\alpha}^{l} v_{z,\alpha}^{m} \right)_{\text{own}} \max(v_{\alpha} \cdot S_f, 0) \quad (4.10)$$

$$+ \sum_{\alpha}^{N} \left( w_{\alpha} \xi_{p,\alpha}^{i} v_{x,\alpha}^{j} v_{y,\alpha}^{l} v_{z,\alpha}^{m} \right)_{\text{nei}} \min(v_{\alpha} \cdot S_f, 0) \quad (4.11)$$

where the subscripts own and nei denote the interpolation from the owner and neighbor cells respectively, and $S_f$ denotes the surface normal vector to the cell face, pointing from the owner to the neighbor cell, with a magnitude of the surface area. This results in a flux contribution from
each quadrature node to the total moment flux. It should be noted that the abscissae are written such that $\xi_{\alpha,\beta,\gamma,\delta} = \xi_{\alpha,\beta,\gamma} = \xi_{\alpha,\beta} = \xi_{\alpha}$, and similarly for the velocity components. While simplifying the storage and calculation of the weights and abscissae, this does add additional field operations. Other techniques such as conditional moment fluxes have been proposed (Fox et al., 2018) but will not be used in this paper due to the added complexity of implementation.

### 4.4.2 Source terms

The source terms that will be examined in the following section are those typical to size distribution evolution, namely aggregation, breakup, and growth or evaporation will follow the formulations seen in Passalacqua et al. (2018) because it has been test and uses the same computational framework where the algorithm proposed in this method is implemented. Additionally, collisional source terms are important when considering the velocity distributions of particulate flows in the non-dilute regimes, where particle interactions are not negligible. The source term for particle-particle interactions is thus written

$$
C(\xi, v, x, t) = B^a(\xi, v, x, t) - D^a(\xi, v, x, t) 
+ B^b(\xi, v, x, t) - D^b(\xi, v, x, t) 
- \nabla_\xi (G(\xi) n(\xi, v, x, t)) + C(\xi, v, x, t),
$$

where $B$ and $D$ are the time rate of change of the number density function due to the birth and death of particles from aggregation and breakup ($a$ and $b$). The growth term has been moved from the left side of the equation to the right so it can be solved in the same manner as the rest of the sources. The final term $C(\xi, v, x, t)$ represents the collisional source.

Following the integration of the GPBE to obtain the moment transport equations the source terms for the moment of order $\{p,i,j,k\}$ are

$$
C_{p,i,j,k}(x, t) = B^a_{p,i,j,k}(x, t) - D^a_{p,i,j,k}(x, t) 
+ B^b_{p,i,j,k}(x, t) - D^b_{p,i,j,k}(x, t) 
- G_{p,i,j,k}(x, t) + C_{p,i,j,k}(x, t),
$$

where

$$
B^a_{p,i,j,k}(x, t) = B^a(\xi_{p,i,j,k}, v, x, t), \\
D^a_{p,i,j,k}(x, t) = D^a(\xi_{p,i,j,k}, v, x, t), \\
B^b_{p,i,j,k}(x, t) = B^b(\xi_{p,i,j,k}, v, x, t), \\
D^b_{p,i,j,k}(x, t) = D^b(\xi_{p,i,j,k}, v, x, t), \\
G_{p,i,j,k}(x, t) = G(\xi_{p,i,j,k}) n(\xi_{p,i,j,k}, v, x, t), \\
C_{p,i,j,k}(x, t) = C(\xi_{p,i,j,k}, v, x, t).
$$
4.4.2.1 PBE source terms

The source terms that will change the particle size are aggregation, breakup, and growth. Because of the very high number density that occurs when very small particles are used, which results in poor conditioning of the Vandermond matrices used to invert the velocity distributions, the source terms have been written using the particle volume fraction as the weight. This is different that other authors Marchisio and Fox (2013); Nguyen et al. (2016) which define the weights in terms of number density. The integral equations are written using the number density formulation, where the approximated summations are written in terms of volume fraction. The change between the two form is done using the relation

\[ n(\xi, v, x, t) = \epsilon(\xi, v, x, t)/\xi^3 \]

and

\[ n_{\alpha} = w_{\alpha}/\xi_{\alpha}^3, \]

where the volume fraction is the third moment of the NDF, i.e. \( M_{p+3,i,j,k}(\epsilon(\xi, v), \xi, v)) = M_{p,i,j,k}(\epsilon(\xi, v), \xi, v)) \).

The growth, or evaporation term is defined as

\[ G_{p,i,j,k}(x, t) = -p \int_{R^+} \int_{R^3} n(\xi, v, x, t)\xi^{p-1}G(\xi)v_x^iv_y^jv_z^k \, dv \, d\xi \]

\[ \approx -p \sum_{\alpha} w_{\alpha}/\xi_{\alpha}^3 v_x^i v_y^j v_z^k G(\xi_{\alpha})\xi_{\alpha}^{p+2}, \] (4.18)

the time rate of change in the birth of particles sizes due to aggregation

\[ B_{p,i,j,k}(x, t) = \frac{1}{2} \int_{R^+} \int_{R^3} n(\xi, v, x, t)\xi^{p-1}v_x^i v_y^j v_z^k \]

\[ \int_{R^+} \int_{R^3} \beta(\xi, \xi') (\xi^{3} + \xi'^{3})^{p/3} \, dv' \, d\xi' \, d\xi \]

\[ \approx \frac{1}{2} \sum_{\alpha} w_{\alpha}/\xi_{\alpha}^3 v_x^i v_y^j v_z^k \sum_{\alpha'} w_{\alpha'}/\xi_{\alpha'}^3 \beta(\xi_{\alpha}, \xi_{\alpha'}) (\xi_{\alpha}^{3} + \xi_{\alpha'}^{3})^{p/3}, \] (4.21)

the time rate of change in the death of particles sizes due to aggregation

\[ D_{p,i,j,k}(x, t) = \int_{R^+} \int_{R^3} n(\xi, v, x, t)\xi^{p-1}v_x^i v_y^j v_z^k \]

\[ \int_{R^+} \int_{R^3} \beta(\xi, \xi') (\xi^{3} + \xi'^{3})^{p/3} \, dv' \, d\xi' \, d\xi \]

\[ \approx \sum_{\alpha} w_{\alpha}/\xi_{\alpha}^3 \xi_{\alpha}^{p+3} v_x^i v_y^j v_z^k \sum_{\alpha'} w_{\alpha'}/\xi_{\alpha'}^3 \beta(\xi_{\alpha}, \xi_{\alpha'}), \] (4.22)
the time rate of change in the birth of particles sizes due to breakup

\[ \frac{D_{p,i,j,k}^b(x,t)}{\partial t} = \int_{\mathbb{R}^3} n(\xi, v, x, t) \xi^p v_i^j v_k^k \]

\[ \approx \sum_{\alpha} \frac{w_\alpha}{\xi_{\alpha}^3} a(\xi_\alpha) \left( b(\xi_\alpha) \right)^{p+3} v_{x,\alpha}^i v_{y,\alpha}^j v_{z,\alpha}^k, \]  

(4.26)

the time rate of change in the death of particles sizes due to breakup

\[ \frac{D_{p,i,j,k}^d(x,t)}{\partial t} = \int_{\mathbb{R}^3} n(\xi, v, x, t) \xi^p a(\xi) v_i^j v_k^k \]

\[ \approx \sum_{\alpha} \frac{w_\alpha}{\xi_{\alpha}^3} a(\xi_\alpha) \xi_{\alpha}^p v_{x,\alpha}^i v_{y,\alpha}^j v_{z,\alpha}^k, \]  

(4.29)

4.4.2.2 Collisional source term

Because of granular cooling rates of a polydisperse system is determined by the mass ratio of the interacting particles (Passalacqua and Fox, 2013), the Boltzmann collision integral is used. The collision source between particle with size \( \xi_\alpha \) and velocity \( v_\alpha \) and a second particle with size \( \xi_\beta \) and velocity \( v_\beta \) is given by

\[ C_{p,i,j,k,\alpha,\beta} = \frac{6\chi_{\alpha,\beta}^2 g_{0,\alpha,\beta}}{d_\beta} \xi_{\alpha}^p \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} I_{i,j,k}^{(0)}(\omega_{\alpha,\beta}, v_\alpha, v_\alpha - v_\beta) \]

\[ |v_\alpha - v_\beta| f_\alpha f_\beta d\xi_\alpha d\nu_\alpha d\xi_\beta d\nu_\beta, \]  

(4.31)

Where \( \chi_{\alpha,\beta} = (d_\alpha + d_\beta)/(2d_\beta) \), \( g_{0,\alpha,\beta} \) is radial distribution function (Carnahan and Starling, 1969; Lun et al., 1984; Ogawa et al., 1980; Sinclair and Jackson, 1989), and the coefficients \( I_{i,j,k}^{(0)}(\omega_{\alpha,\beta}, v_\alpha, v_\alpha - v_\beta) \) are defined in Marchisio and Fox (2013). Here, \( \omega_{\alpha,\beta} \) is a function of the two particle masses and the coefficient of restitution \( e_{\alpha,\beta} \) and is defined as

\[ \omega_{\alpha,\beta} = \frac{m_\beta(1 + e_{\alpha,\beta})}{m_\alpha + m_\beta}. \]  

(4.33)

Other methods such as an extension to a multiple size BGK/es-BGK model has been described in Marchisio and Fox (2013), but have been shown to be insufficient to describe granular cooling for polydisperse systems (Passalacqua and Fox, 2011).
Unlike the monodisperse case, where the collisional source terms of the BGK/es-BGK models can be solved implicitly (there is no implicit form for the full Boltzmann collision model), the polydisperse formulation does not allow for this, requiring an explicit method to be used in order to integrate the collisional sources.

4.5 Numerical procedure

The approach described in the previous sections was implemented in the OpenQBMM framework (Passalacqua et al., 2018), a derivative of the OpenFOAM toolbox (OpenCFD Ltd., 2018). The solution to the moment transport equations is using operator splitting for advection, acceleration terms, and population balance and collisional source terms. By doing this, moment realizability can be ensured at each operator split. In addition, it also allows more numerically stable approaches to be taken especially in regards to the solution of acceleration terms (specifically drag) acting on the velocity abscissae.

When time scales associated with the source terms are very small compared to the advection time scales, the source must be handled so that it does not cause moment sets to become unrealizable. To alleviate this the realizable RK2-SSP ode solver of (Nguyen et al., 2016) is used to integrate the entire moment set each time step by ensuring both accuracy and moment realizability.

1. First we begin by updating the moments due to advection, solving

\[
\frac{\partial M_{pijk}}{\partial t} + \nabla \cdot F_{pijk} = 0.
\] (4.34)

The quadrature is then updated ensuring that the entire moment set is realizable.

2. Next, the moments are updated using a realizable RK2-SSP ode solver described in Nguyen et al. (2016)

\[
\frac{\partial M_{pijk}}{\partial t} = C_{pijk}.
\] (4.35)

The quadrature is again updated and moment realizability is checked.
3. Finally, because the size distribution is not changed by the acceleration terms acting on the size-velocity distribution \((w_\alpha, \xi_\alpha)\), the change in the velocity abscissae due to these forces is solved

\[
\frac{\partial v_\alpha}{\partial t} = A(\xi_\alpha, v_\alpha) + g. \tag{4.36}
\]

The moment set is updated using the new velocity abscissae.

4. Advance in time a return to step 1.

### 4.6 Results

The verification of the inversion procedure and numerical method will be done in four parts. First, the time integration of source terms is validated using 0-D test cases for population balance source (Passalacqua et al., 2018) and polydisperse collisional source terms (Passalacqua and Fox, 2011). Secondly, the method will be applied to a collection of polydisperse droplet cases (Fox et al., 2008). Third, the ability to handle crossing jets with particles of multiple sizes is examined, showing that multiple particle velocities can exist in a single cell. This is unique from the standard hydrodynamic equations due to the fact that only one mean velocity is used to transport the conserved quantities and the equal and opposite momenta cancel one another out due to a zero mean velocity. Lastly, 2-D cases will be used to validate the ability of the method to handle crossing dilute particle jets, and the ability for multiple velocities to exist in one computational cell.

#### 4.6.1 Validation of source terms

The validation of the source terms, aggregation, breakup, and collisions, will be validated using 0-D cases. These cases will make use of an adaptive time stepping ODE solver described in Nguyen et al. (2016). The Boltzmann bidisperse collisional model is validated using comparisons of equilibrium temperature ratios of a bidisperse mixture to that of theoretical results as well as molecular dynamics simulations (Dahl et al., 2002). The aggregation and breakup sources are validated using case 5 from Passalacqua et al. (2018).
4.6.1.1 Aggregation breakup

Pure aggregation and breakup cases are used to validate the respective source terms, however the velocity distributions are prescribed with zero mean and unit variance to ensure that quadrature algorithm is tested. Cases 5, 6, and 7 from Passalacqua et al. (2018) are used, and Fig. 4.1 shows that results exactly reproduce the previous univariate results. A global time step of 1 s is used, however the time step is adapted within the ode solver to ensure moment realizability and accuracy. The cases took a total time of 1460 s, 1600 s, and 2116 s respectively on a single core of a dual Intel Xeon CPU Intel® Xeon® CPU E5-2667 v3 at 3.20 GHz. While these times are significantly longer than is required for the univariate cases, they are merely meant to illustrate the accuracy of the integration method.
4.6.1.2 Bidisperse granular cooling

The Homogeneous cooling of particle with different diameters is used to test the implemented Boltzmann collision integral by comparing the steady state ratio of temperatures of larger and smaller particles. These results are compared to molecular dynamics simulations and exact solutions to the Enskog solution (Dahl et al., 2002). The results match the exact solution, however there is still deviation at lower values of the coefficient of restitution, likely due to the need of higher order moments to accurately capture the evolution temperature ratio.

4.6.1.3 Droplet Evaporation and Coalescence

A common application of the general population balance equations is that of droplet coalescence, breakup, and evaporation. The presented results are compared to that of Laurent et al. (2004); Fox et al. (2008). The comparison results were obtained using the direct quadrature based method of moments. The case set up is presented in Laurent et al. (2004) and is solved assuming that the droplets do not effect the fluid flow. The fluid velocity is defined as

\[ U_z = \frac{z_0^2 V(z_0)}{z^2}, \quad (4.37) \]
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<table>
<thead>
<tr>
<th>$N_{\xi}$</th>
<th>$w_{\alpha}/\varepsilon_l$</th>
<th>$\xi_{\alpha}$ [$\mu$m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.00625e-3</td>
<td>8.81592</td>
</tr>
<tr>
<td>2</td>
<td>0.276135</td>
<td>22.0820</td>
</tr>
<tr>
<td>3</td>
<td>0.612420</td>
<td>36.5680</td>
</tr>
<tr>
<td>4</td>
<td>0.105439</td>
<td>56.7900</td>
</tr>
</tbody>
</table>

Table 4.1 Inlet conditions initial size distribution for monomodal cases.

\[ U_r = r \frac{z_0^2 V(z_0)}{z^3}, \]  

(4.38)

where $U_\alpha$ is the flow velocity along the primary injection axis, $U_r$ is the radial velocity, $z_0$ is the position of the nozzle inlet, $r$ is the radial position, and $V(z_0)$ is the inlet nozzle velocity. This configuration leads to straight streamlines for both the gas velocity and particle velocity. The comparison of the volume fraction, $M_{000}$ or $\varepsilon_l$, and relative velocity magnitude are presented for three cases using a monomodal size distribution with $z_0 = 10$ cm and $V(z_0) = 5$ m/s: a) linear evaporation with no coalescence, b) non-linear evaporation with no coalescence, and c) non-linear evaporation linear evaporation with shear driven coalescence. Due to the fact that the presented model uses volume fraction for the zero order moment, the initial weights and diameters have been converted from the number density description in Fox et al. (2008) to the volume fraction description and can be seen in Table 4.6.1.3. A final case using a bimodal size distribution with $z_0 = 5$ cm and $V(z_0) = 5$ m/s, droplets with sizes 10 and 30 $\mu$m with equal volume fractions, and non-linear evaporation with no coalescence is presented. All cases have droplet inlet velocities equal to the gas velocity, inlet volume fraction of $\varepsilon_l = 0.0057$, and use four nodes to represent the size distribution, resulting in a total of 36 quadrature nodes (nine for each size-conditioned velocity distribution). The models used are presented in Fox et al. (2008).

Because the zero-size evaporation flux is zero when the linear evaporation model is used, the results match the previous DQMOM results exactly (Fig. 4.3). However, because the zero-size flux is not zero for the non-linear model and the ability of the presented method to adapt the quadrature when droplet sizes disappear, the results differ when the zero-flux is included and when it is not in the DQMOM approach (Fig. 4.4). The adaptive quadrature used in the present method is also
Figure 4.3  Monomodal distribution with linear evaporation and no coalescence.

Figure 4.4  Monomodal distribution with non-linear evaporation and no coalescence.

Figure 4.5  Monomodal distribution with linear evaporation and coalescence.
likely the reason of the difference between the location of the peak in mass density when compared with the results of DQMOM. When coalescence is included the mass density profile matches quite well, but the relative velocity deviates due to the fact that more quadrature nodes are used in the comparisons results of DQMOM (8 size nodes (Fig. 4.5). Currently, the standard QMOM inversion process is limited to 5 nodes due to numerical complications that arise in the definition of higher order moments. Using the extended quadrature method of moments (Yuan et al., 2014) is able to alleviate this problem by more accurately representing the size distribution evolution using a smaller number of nodes, but will not be examined in this paper. The final, bimodal case, shows excellent comparison to the DQMOM results using no zero-flux (Fig. 4.6). In order that they have been presented, the run times of the simulations are 36 minutes, 26 minutes, 14 hours, and 32 minutes. The case including coalescence takes so much longer due to the fact that the coalescence source terms are dependent on the entire velocity distributions, and there for it requires an $N^2$ operations at each local time step. It should also be noted that a monokinetic approximation of the distribution is sufficient due to the low Stokes number of the droplets, but like the 0-D size evolution cases has been included to validate the method. An additional factor in the increased runtimes in comparison with Fox et al. (2008) is that while additional transport equations are solved, the solution is also evolved in time until a steady state is reached instead of solving the steady weight and abscissae transport equations.
4.6.1.4 2-D Jet Crossing

One major advantage of using quadrature based moment methods is that the entire velocity distribution is used to advect the NDF allowing particle trajectories to cross when the VDF is not a delta distribution. By using size-conditioned velocity distributions even conditional VDF represented only by a mean (monokinetic) trajectories are able to cross. However when particles have a large Stokes number, even particles of the same size may have trajectories that cross. The capability of describing this phenomena is a key advantage of using CHyQMOM. In order to illustrate this ability, two cases of crossing jets are presented. The first being a dilute case where there are no collisions between particles. In this case, particle trajectories should pass through one another while maintaining a constant velocity distribution. In addition to the velocities, the sizes should also be constant. Three inlets are used where the particle sizes are 1 mm and 2 mm, 2 mm and 3 mm, and 3 mm and 1 mm from left to right. A reflective wall boundary condition (Struchtrup, 2005) is used on the left, right, and bottom boundaries and a zero gradient outlet condition is used on the top. The computational domain can be seen in Fig. 4.7.
Table 4.2  Inlet conditions of inlets 1, 2, and 3 as well as the number of size nodes used in each test case. The particle sizes are denoted as S for small (1 mm), M for medium (2 mm), and L for larger (3 mm).

<table>
<thead>
<tr>
<th>Case</th>
<th>Inlet 1</th>
<th>Inlet 2</th>
<th>Inlet 3</th>
<th>N-size nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>M</td>
<td>-</td>
<td>M</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>M</td>
<td>M</td>
<td>M</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>S, M</td>
<td>-</td>
<td>S, M</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>S</td>
<td>M</td>
<td>L</td>
<td>3</td>
</tr>
<tr>
<td>5</td>
<td>S, M</td>
<td>M, L</td>
<td>S, L</td>
<td>3</td>
</tr>
</tbody>
</table>

The results of case 1 show that in the monodisperse limit two crossing jets pass through one another with no change in the velocities, Fig. 4.8. Case two shows the limitations in the inversion process used to invert the conditioned velocity moments in that when three particle trajectories cross at a given point, the resulting velocity abscissae are corrupted, Fig. 4.9. In order to correctly predict this flow, additional velocity nodes must be used in the inversion process. When multiple sizes are used, it allows for additional information to be gained in regards to the velocity distribution such that three trajectories can cross without corrupting the reconstructed distribution. It should be noted that assuming a mono-kinetic size-velocity distribution (one velocity per size, or one velocity node) would accurately predict this crossing as well. Fig. 4.10 shows two streams with two sizes per stream, Fig. 4.11 shows 3 streams, each with a unique size, and Fig. 4.12 shows three streams with overlapping sizes.
Fig. 4.8 is meant to show that in the monodisperse limit, the two jet streams can still cross without numerical problems. This is the same as only solving for a velocity distribution without size conditioning.

Fig. 4.9 shows the numerical limits of the velocity distribution algorithm in which at most two crossing jets is the most that can be correctly solved. When three jets cross, a higher number of nodes is required to accurately represent the cells in which this occurs.

Fig. 4.10 shows the bidisperse case in which two jets, each with equal volume fractions of two unique sized particles cross. The result is the same as in case 1, showing that the size conditioning step does not contaminate the velocity distribution.

Fig. 4.11 shows three jets, each with a unique size crossing at one point. Unlike case 2 this is possible because each size carries its own velocity distribution allowing for as many streams to cross as there are size nodes with unique sizes. For this specific case, the use of CHyQMOM is actually unnecessary, and the flow can be correctly solved for using a monokinetic approximation similar to (Heylmun et al., 2019) due to the fact that each size only requires one velocity per cell to reconstruct the full distribution.

It can be seen in the contours of the particle diameters in Fig. 4.12 that the mean diameter has some fluctuations unlike the previous cases in which a constant mean diameter existed in the respective streams. This is due to the fact that the conditional moment inversion does not guarantee that the size conditioned velocity moments are fully realizable and therefore numerical
(a) Volume fraction
(b) Mean x-velocity
(c) Mean diameter
(d) Standard deviation of diameter

Figure 4.10  Two bidisperse crossing jets

Figure 4.11  Three crossing jets, each with a unique size
errors can cause velocity abscissae to different between sizes. This leads to different moment fluxes and therefore a non-constant mean diameter profile.

A second case is presented where particle collisions using the Boltzmann collision are presented in Fig. 4.13. The same computational domain and boundary conditions are used as the case prior. While both inlets will have the same mass flow rate, the left will have a diameter of 100 µm and the right of 300 µm. The change to a non-symmetric flow pattern is produced by the increased number of collisions and therefore a higher dissipation of granular temperature in the smaller particle size. This results in the momentum of the larger particles dominating that of the smaller particles. The plots of granular temperature and velocity covariance are shown in Fig. 4.13 to emphasize the importance of the higher order statistics in the velocity distributions to predict flow patterns, especially in the dilute regime.
Figure 4.13  Two crossing jets using source terms for collisions
4.7 Conclusions

A novel method for obtaining the solution to the evolution of the four dimensional, size-velocity NDF transport has been presented and validated using simple and real test cases. The presented model has been derived from the number density function evolution equation, and the relevant source terms have been modified to allow for the volume fraction based definition of the moments. The source terms were validated using 0-D cases for both pbe (Passalacqua et al., 2018) and bidisperse collisions (Dahl et al., 2002) and match previous results obtained from both exact and numerical solutions. The combination of advection and changes in size was then validated using a collection of 1-D axisymmetric spray cases. When a sufficient number of nodes was used, the results match quite well in comparison to the previous results of Fox et al. (2008). Finally, a collection of jet crossing cases were presented to illustrate the capabilities as well as the limitations of the inversion process in regards to multiple particle velocities within a control volume.

4.8 References


CHAPTER 5. SUMMARY AND DISCUSSION

This thesis has been intended to present new methods for simulating multiphase flows using moment methods. These new approaches have been validated using previous methods, while allowing new regimes of problems to be examined.

In Chapter 2 a new method to couple the standard two-fluid model to quadrature based moment methods was developed allowing for both the high and low volume fraction limits to be represented correctly. The methods make use of standard numerical techniques to ensure a stable solution allowing for difficult cases to be simulated. The presented algorithm was validated using a merging 1-D size distribution where the solution became grid independent showing that the system of equations is hyperbolic. The method was also shown to reproduce the two-fluid model when in the monodisperse limit, and reproduce the multi-fluid model when fixed bubble sizes are used. The simulation of oscillation frequency was also validated against experimental data, and showed good agreement. Finally the model was stress-tested using an unstructured mesh with high superficial gas-velocity, illustrating the model's stability.

In Chapter 3 standard kinetic theory numerical techniques were modified so that they can be used in polydisperse systems while still ensuring conservation of mass. This modified algorithm limits the flux due to the granular and frictional pressures of a solid phase, and ensuring that both local and total solid volume fraction limits are not surpassed through the use of the MULES flux limiter. The results are shown to be qualitatively accurate for settling bed, while also showing good quantitative agreement with previous implementations and experiments. The final case, that of a cyclic riser showed good agreement for the spatial distribution of small particles while over predicting the concentration of larger particles at the walls. This is likely due to the cyclic nature of the simulation.
Finally, in Chapter 4 a novel method for the simulation of a joint size-velocity distribution using quadrature based moment methods was presented. An improved inversion algorithm was presented which takes advantage of the accuracy and stability of an analytical solution for the inversion of the conditional velocity moments. The volume fraction based representation of the NDF was presented allowing for the stable transport and evolution of micrometer size particles. The method was validated using 0-D evolution cases with contributions from size and collisional source and the results matched analytic results very well. A collection of 1-D spray simulations were then conducted, showing that when the distribution is sufficiently resolved the method is able to accurately reproduce the results obtained with Lagrangian simulation and the DQMOM method. Finally a collection of 2-D crossing jet cases were presented showing the ability of the inversion algorithm to handle multiple sizes and velocities within a single cell.
APPENDIX RESSUBSTITUTION STEP FOR THE N-PHASE PARTIAL ELIMINATION ALGORITHM

An optional extension of the partial elimination step in the solution to the pressure-velocity system of equations is to estimate the phase velocities only using the phase velocity under consideration. For two phases this process can be completed using a simple algebraic manipulation. However, for n-phases, this becomes a system of n-linear systems which becomes increasingly complex as the number of phases increases. This system can be written as

\[
\mathbb{K} \mathbf{V} = \mathbf{S}, \quad (1)
\]

or

\[
\mathbf{V} = \mathbb{K}^{-1} \mathbf{S}, \quad (2)
\]

where \( \mathbb{K} \) is the matrix of drag coefficients, \( \mathbf{V} \) is the vector of phase velocities, and \( \mathbf{S} \) is the vector of momentum sources, neglecting the pressure gradient terms. The matrices and vectors are defined as

\[
\mathbb{K} = \begin{bmatrix}
\lambda_1^{-1} & K_{12} & K_{13} & \cdots & K_{1n} \\
K_{21} & \lambda_2^{-1} & K_{23} & \cdots & K_{2n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
K_{n2} & K_{n2} & K_{n3} & \cdots & \lambda_n^{-1}
\end{bmatrix}, \quad (3)
\]

\[
\mathbf{V} = \begin{bmatrix}
U_0^1 \\
U_0^2 \\
\vdots \\
U_0^n
\end{bmatrix}, \quad (4)
\]
where the final element in Eq. 5 is only used for phases with a phase pressure (or particle pressure).

Solving this linear system results in an estimation of the phase velocities which then need to be corrected using the solution of the pressure equation

\[ U_i = V_i - \alpha_i \nabla p. \]