On Spray Modeling with Quadrature-Based Moment Methods

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Spray modeling requires a proper representation of the dispersed phase and involves models for a variety of physical phenomena. On the population scale, a properly formulated population balance equation provides a complete statistical description of the particle system. However, in most cases the high dimensionality entails prohibitive computational costs. Quadrature-based moment methods (QBMM) limit the description of particle populations to a set of only a few moments and thus considerably reduce computational complexity. In order to apply QBMM to sprays, models for many involved physical processes must be formulated consistently in the QBMM-context. We study secondary droplet breakup with QBMM using a simple well-established spray breakup model and simplified setups.

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1 Introduction

The numerical simulation of sprays, i.e., an ensemble of fine droplets dispersed in a gaseous carrier phase, is particularly challenging in several ways. One important aspect is the representation of the dispersed phase and its interaction with the continuous phase. On the population scale, the number density function (NDF) with respect to a set of characteristic internal coordinates can provide a complete statistical description of the dispersed phase. Its evolution in time, physical space and phase (internal coordinate) space is then governed by a population balance equation (PBE). However, the high dimensionality normally entails prohibitive computational costs using standard discretization methods. Quadrature-based moment methods (QBMM) reduce the representation of the dispersed phase to a set of only a few moments. The governing moment transport equations are derived from the PBE and require closure which is obtained by utilizing Gaussian quadratures rules. This allows the use of only a few discrete points in phase space while maintaining maximum accuracy with respect to the integral terms, i.e., the moments.

Another key aspect of spray modeling is the development of physical models for all involved processes, one of which is the breakup of larger drops into smaller drops, also referred to as secondary breakup. A variety of breakup models for PBEs exist [1]. They are however almost exclusively suitable for bubble flows as they consider collisions with turbulent eddies in the heavier surrounding fluid to be the dominant mechanism, whereas the fragmentation of liquid drops is primarily controlled by growing surface instabilities in most breakup regimes (e.g., [2]). We employed the relatively simple and well-established spray breakup model by Reitz and Diwakar [3], formulated here for QBMM.

2 Governing Equations

Presuming a spatially homogeneous system and the absence of all physical effects other than breakup, the PBE governing the evolution of the NDF \( n(t, \xi) \) reduces to the fragmentation equation

\[
\frac{\partial n(t, \xi)}{\partial t} = -\nu(\xi)n(\xi) + \int_{\xi}^{\infty} \nu(\xi') \beta(\xi | \xi') n(\xi') d\xi',
\]

where \( \xi \) denotes some measure of drop size, \( \nu(\xi) \) the breakup frequency of droplets with size \( \xi \) and \( \beta(\xi | \xi') \) the conditional size distribution function of daughter droplets given parent droplets of size \( \xi' \). Physically interpreted, the first term on the right-hand side of Eq. (1) accounts for the disappearance of parent droplets and the second term for the formation of new daughter droplets.

A main feature of QBMM is the representation of the dispersed phase by a finite set of moments. With the definition of the moment of \( k \)th order

\[
m_k(t) = \int_{\Omega_\xi} \xi^k n(t, \xi) d\xi
\]

the fragmentation equation (1) can be transformed into a set of ordinary differential equations. After some rearrangements and application of the quadrature method of moments (QMOM) [4], one specific type among the different QBMM [5], the

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temporal change of the $k$th moment can be expressed as

$$\frac{d m_k(t)}{dt} \approx \sum_{\alpha=1}^{N} w_\alpha \nu(\xi_\alpha) \left[ \int_0^{\xi_\alpha} \xi^k \beta(\xi) d\xi - \xi^k_\alpha \right],$$

where $\xi_\alpha$ and $w_\alpha$ are the abscissas and weights of an $N$-node quadrature, respectively.

The breakup rate $\nu(\xi)$ and daughter distribution function $\beta(\xi')$ were determined based on the relationships described by Reitz and Diwakar [3], formulated consistently with QBMM. However, a major difference from the original model remains: In the original model formulation daughter drop sizes at time $t + \Delta t$ are determined by solving a rate equation $d\xi/dt = f(\nu(\xi), \beta(\xi'))$, presumably due to the practical limitations on the number of particles in Eulerian-Lagrangian spray simulations. QBMM do not have such limitations. Hence, the discontinuous disintegration process as described in the fragmentation equation (1) can be realized without any additional computational costs.

### 3 Results

First investigations were carried out on a spatially homogeneous system without momentum exchange and with droplet diameter as the only internal coordinate ($\xi \equiv d$). Initial droplet sizes are log-normally distributed with a mean of 20 $\mu$m and a standard deviation of 8 $\mu$m. Using constant thermophysical properties of iso-octane and air at a temperature of 293 K yields Weber numbers up to 175, Reynolds numbers up to 1825 and Ohnesorge numbers up to 0.018 (as the log-normal distribution has the support $(0, \infty)$, the maximum diameter $d_{\text{max}}$ to calculate the characteristic dimensionless numbers was chosen to be the one where $d \leq d_{\text{max}}$ is true for 99% of the droplets).

The standard QMOM was employed with different numbers of quadrature nodes. Fig. 1 shows results of QMOM simulations as well as Monte-Carlo simulations using the original model with the above-mentioned rate equation and also a modified model equivalent to the fragmentation equation (1) to enable verification of the results. In general, the results indicate that improvements in accuracy with an increasing number of quadrature nodes become negligible if $N \geq 3$.

Moreover, it is revealed that the model with a discontinuous formulation, which is in principle closer to the real fragmentation process, yields much more rapid atomization. This results in a faster increase of number concentration and a faster decrease in the Sauter mean diameter, suggesting quick relaxation of the system in the presence of drag, heating and vaporization and consequently enhanced momentum, heat and mass transfer.

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