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Solution of population balance equation using quadrature method of moments with an adjustable factor

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Abstract

For description of dispersed phases in many practical applications, population balance equations (PBE) of entities under investigation are coupled with the thermo-fluid dynamics of the surrounding fluid. Hence, solution of PBE needs to be implemented in a computational fluid dynamics (CFD) code, which leads to additional computational cost. The excess computational demand has limited the applicability of numerical techniques such as class method (CM) or Monte Carlo method (MCM). Although quadrature method of moments (QMOM) and direct quadrature method of moments (DQMOM) have been shown to be accurate and computationally efficient when used with CFD codes, numerical difficulties can arise for cases where there is a large variation of moments. To circumvent this problem, the standard QMOM was modified by incorporating an adjustable factor, which allows the moments of size distribution to be adjusted, in order to improve the accuracy or reduce CPU time. The performance of this method for solving PBE has been evaluated by case studies involving pure aggregation and breakage, agglomeration and breakup, as well as particle growth, which have analytical solutions or exact solutions from CM or finite element method (FEM). The results demonstrate that the modified QMOM is capable of achieving high accuracy at a low CPU cost if an appropriate adjustable factor is chosen. An interesting feature is that different adjustable factors can be assigned to different processes depending on the balance between accuracy requirement and CPU cost.

Keywords: Population balance model; Quadrature method of moments (QMOM); Dispersed system

1. Introduction

Dispersed system is encountered in many industrial processes. The behavior of dispersed systems such as gas–liquid or liquid–liquid systems depends strongly on the flow characteristics of the dispersed phase. Distribution of the dispersed phase size and different particle or bubble shapes may alter the flow pattern considerably. The effect of dispersed phase size distribution cannot be taken into account by using a single mean size of the dispersed phase in two-fluid models. Therefore, population balance model is employed to describe the distribution of entities (e.g. bubble, particle and drop) and their micro-behaviors (breakage or coalescence) which affect the distribution.

The distribution of entities depends not only on space and time referred as external coordinates but also their own properties referred as internal coordinates. The micro-behavior can be divided into continuous behavior (particle growth or dissolution) or discontinuous behavior (bubble breakage or coalescence). Population balance equations (PBE) contain external time and location coordinates as well as internal entity property coordinates, the source term of which usually involves single or multi-integrals. As the form of PBE is very complex and analytical solutions are available only for the simplest cases, numerical techniques are required in most practical applications. Such techniques should be accurate and with a relatively low computational cost. Several

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numerical methods have been developed to satisfy the accuracy requirement, among which are class method (CM) (Kumar and Ramkrishna, 1996a, b; Vanni, 2000), Monte Carlo method (MCM) (Smith and Matsoukas, 1998; Tandon and Rosner, 1999) and method of moment (MOM) (McGraw, 1997; Rong et al., 2004). In the CM, the continuous size range of the internal coordinate is partitioned into a finite series of contiguous subintervals or bins. Good accuracy can be achieved if a large number of size groups are used, but at the expense of high CPU cost due to increased number of scalars to be solved. The number of classes is a potential problem in computational fluid dynamics (CFD) applications, especially when a multi-fluid flow model needs to be used; hence the CM method is not a feasible approach in practice. MCM is based on the solution of PBE in terms of its stochastic equivalent. A population of particles undergoes the "real" physical processes, and events occur according to the appropriate probabilities. In order to reduce the statistical error, a very large number of particles must be used. Due to limitations on the computational resources, the full incorporation of MCM into CFD codes is still intractable (Rong et al., 2004). In MOM, the particle size distribution (PSD) is not tracked directly but through its moments integrated over the internal coordinates. This approach has many advantages such as low CPU time and relatively high accuracy. The standard method of moment (SMM) needs to be closed, which limits its practical application. McGraw (1997) introduced the Gaussian quadrature approximation for PSD which closes the SMM, and proposed quadrature method of moments (QMOM). QMOM has been widely used for PBE in recent years (Marchisio et al., 2003a, b; Wang et al., 2005a, b), and has been extended to bivariate PBE applications (Wright et al., 2001, Yoon and McGraw, 2004a, b). However, this approach is difficult to handle systems where there is a strong dependence of the dispersed-phase velocity on internal coordinates (e.g. fluidized bed and bubble column), and can become quite complex in the case of bivariate PBE (Marchisio and Fox, 2005). Although the direct quadrature method of moments (DQMOM) was proposed by Rong et al. (2004), which can be extended to multi-variable application in a straightforward manner (Rong et al., 2004) and has considered different characteristic lengths with different velocities. Because DQMOM uses different phases to distinguish characteristic lengths, hence is more time-consuming than QMOM when coupled with CFD.

Previous studies have shown that the accuracy and time consumption of MOM depend largely on the relative magnitude of the moments. The matrix becomes extremely difficult to solve if the moments vary over a large range. In such cases, solution of differential equations and product-difference (PD) algorithms in QMOM or matrix inversion in DQMOM would require excessive computational resources. When the source term of PBE is too large, negative weights or abscissas may appear in the simulations, which do not have physical meaning and will result in abortion of the computation. This potential problem can be avoided if the moments could be modified in a controlled manner. To serve this purpose, a modified QMOM has been developed. In the new method presented here, the variation among the moments can be controlled by an adjustable factor. A number of test cases have been carried out, including breakage, aggregation and growth of entities to evaluate the performance of this method for PBE.

2. Population balance model and solution

2.1. Population balance model

In order to describe the PSD in a certain system, internal and external coordinates, which are referred as entity state space, must be employed. Number density function (NDF) is commonly used to describe this distribution in the state space. NDF can be defined in several ways depending on the properties of the system concerned. Given the coordinates of the property vector $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)$ that specify the state of the entity, the NDF $f(\xi_1, \ldots, \xi_N; \mathbf{x}, t)$ is defined as follows (Marchisio et al., 2003b):

$$f(\xi_1, \ldots, \xi_N; \mathbf{x}, t)\,\mathrm{d}\xi_1, \ldots, \mathrm{d}\xi_N = f(\xi; \mathbf{x}, t)\,\mathrm{d}\xi, \tag{1}$$

which represents the number of entities with a value of the property vector between $\boldsymbol{\xi}$ and $\boldsymbol{\xi} + \mathrm{d}\boldsymbol{\xi}$ at time t and location $\mathbf{x}$. Eq. (1) may have different forms depending on the entity property. As single length property is considered in this paper, the property vector $\boldsymbol{\xi}$ becomes a scalar, L.

PBE is a continuous statement of NDF. If single characteristic length property is considered, PBE can be defined as

$$\frac{\partial f(L; \mathbf{x}, t)}{\partial t} + \frac{\partial}{\partial x_i}(\langle \mathrm{u}_i \rangle_L f(L; \mathbf{x}, t)) = S(L). \tag{2}$$

Eq. (2)conforms to the Einstein sum assumption, where $f(L; \mathbf{x}, t)$ is the NDF; $\langle \mathrm{u}_i \rangle_L$ is the entity mean velocity conditioned on property value L at i direction; $S(L)$ is the source term of PBE, which is related to micro-behaviors in a dispersed system.

Eq. (2) is the transport equation for NDF, and the source term usually presents itself in single integral, multi-integral or differential forms.

2.2. Adjustable moment of entity and characteristic parameters in a poly-dispersed system

In MOM, entity PSD is not tracked directly, but through its moments integrated over the internal coordinate. In order to adapt the moment according to a certain PSD, adjustable moment of the entity PSD is defined as follows:

$$m_k(t) = \int_0^\infty L^{k/p} f(L; t)\,\mathrm{d}L, \tag{3}$$

where $m_k(t)$ is an adjustable moment of the PSD; $f(L; t)$ is the NDF of characteristic length L and p is the adjustable factor ($p = 1$ is equivalent to the standard QMOM). The adjustable moment m_k has different physical meanings depending on the relation of k and p. If $k = 0$, $m_0(t)$ is the total number of entity considered; when $k = 2p$, $m_{2p}(t)$ is related to the total area ($A_t = k_A m_{2p}$) of all the entities; when $k = 3p$, m_{3p} is related to the total volume ($V_t = k_v m_{3p}$). The shape factors k_A and k_v