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Multivariate Quadrature-Based Moments Methods for turbulent polydisperse gas–liquid systems

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ABSTRACT

The Conditional Quadrature Method of Moments (CQMOM) and the Direct Quadrature Method of Moments (DQMOM) are compared with Direct Simulation Monte Carlo (DSMC) for the description of gas bubble coalescence, breakage and mass transfer with the surrounding continuous liquid phase. CQMOM and DQMOM are both moment methods based on the idea of overcoming the closure problem by using a quadrature approximation. The methods are compared and performances evaluated for spatially homogeneous and inhomogeneous systems. Eventually CQMOM and DQMOM are implemented in a commercial CFD code to simulate a realistic two-dimensional bubble column. Particular attention is paid to the impossibility of conserving moments with DQMOM in the presence of numerical diffusion. To cure this problem a fully-conservative DQMOM formulation is presented and tested. The relationship between the two methods is investigated, showing that under particular conditions CQMOM is identical to DQMOM. The different methods are employed under a number of different conditions including very fast chemical reactions, in order to highlight if the problem of bubble coalescence, breakage and mass transfer really needs a bivariate population balance to be tackled and what is the optimal number of nodes for the quadrature approximation.

1. Introduction

Disperse systems are usually characterized by complex interactions between the continuous phase and the disperse phase, and between the different particles/elements constituting the disperse phase. These interactions can be classified as continuous or discontinuous depending on the time and spatial scale chosen to observe the system: a continuous process will result, considering an infinitesimal time scale, in an infinitesimal change of properties of the dispersion, otherwise a discontinuous event brings to a finite change of the system status. The Generalized Population Balance Equation (GPBE), the mathematical framework used to describe these systems, is a generalization of the classical Population Balance Equation (PBE) (Ramkrishna, 2000), that tracks their evolution not only in physical space, but also in the space of the properties of the population (called internal coordinates). We are interested in analyzing different approaches, capable of describing industrial scale systems characterized by strong spatial heterogeneity and a high degree of poly-dispersity in the internal coordinates with an optimal balance between accuracy and computational costs. In this work the focus in on gas–liquid reactors and bubble columns.

Most of the developed methods for solving the population balance equation belong to one of the following groups: classes or sectional methods, Monte Carlo methods and moment-based methods. The first group contains all those methods in which the space of internal coordinates is discretized: the Classes Methods (CM) were firstly developed for the solution of univariate cases, in which the state of the population is characterized by a single property or variable (Kostoglou and Karabelas, 1994; Vanni, 2000) and were recently extended to multivariate cases, in which two or more variables are needed for describing the disperse system (Kumar et al., 2008; Nandanwar and Kumar, 2008). The main drawback of these methods is the high computational costs required to obtain an acceptable accuracy, when also the inhomogeneities in the physical space are taken into account. It is worth mentioning that Finite Volume Methods (Gunawan et al., 2004) and Finite Element Methods (Godin et al., 1999) belong to the group of classes methods and hence they, too, show the aforementioned limitations in the applicability to realistic inhomogeneous cases.

Monte Carlo Methods (MCM) are based on the solution of stochastic differential equations that are able to reproduce a finite number of artificial realizations of the system under investigation (Zhao et al., 2007). In order to have a solution very close to reality, the number of artificial realizations is often very high, resulting in unsustainable computational costs. For this reason, these methods

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are usually employed for validation (Zucca et al., 2007) in simplified cases.

The Method of Moments was originally formulated and applied to particulate systems in the pioneering work of Hulburt and Katz (1964). The idea behind this method is the integration of the PBE in the space of the internal coordinates, leading to a set of equations that can be solved only for some lower-order moments. For realistic processes, it is not always possible to write the governing equations in terms of the moments themselves, generating what is known as "closure problem"; many closures were proposed in order to overcome this issue and our work is focused on a particular class of methods called Quadrature-Based Moments Methods (QBMM), in which the Number Density Function (NDF) representing the population is assumed to be a summation of some basis function (very often Dirac delta functions) centered on the zeros of orthogonal polynomials of a Gaussian Quadrature. Although the quadrature approximation is always very accurate comparison with alternative methods (Marchisio et al., 2003b; Zucca et al., 2007) is always suggested. In general, acceptable accuracy can be achieved with a very low number of nodes ($N \leqslant 4$) (Marchisio et al., 2003b; Marchisio and Fox, 2005). Moreover, the great advantage is that QBMM are particularly suitable to be coupled with CFD solvers, as demonstrated by Marchisio et al. (2003a), Fan et al. (2004), Zucca et al. (2006), Petitti et al. (2010), and Buffo et al. (2012).

QBMM can be subdivided into two main groups: in the former the evolution of moments is calculated and the quadrature approximation is determined through a specific inversion algorithm; in the latter the quadrature (in terms of its weights and nodes) is directly evolved in space and time by mimicking the evolution of some moments. For univariate PBE, these two methods correspond to the Quadrature Method of Moments (QMOM) (McGraw, 1997) and to the Direct Quadrature Method of Moments (DQMOM) (Marchisio and Fox, 2005), respectively. For multivariate PBE, as reported in Marchisio and Fox (2005), DQMOM can be easily extended, while QMOM, with its standard inversion algorithms, cannot be used as it is not capable of dealing with mixed moments, that arise from multivariate populations. Among the recently proposed inversion algorithms for multivariate problems (Brute-Force, Wright et al. (2001), Tensor Product, Yoon and McGraw (2004a), Yoon and McGraw (2004b), and Fox (2009a) and Conditional Quadrature Method of Moments, CQMOM, Yuan and Fox (2011)) CQMOM was proved to perform excellently. In this work, CQMOM will be compared to DQMOM in order to highlight the pros and cons of each method and establish the better procedure for highly heterogeneous and poly-disperse realistic gas–liquid systems.

As far as the coupling to Computational Fluid Dynamics (CFD) codes is concerned, some issues for both methods still need to be addressed. As it is well-known, "moment-corruption", namely the generation of invalid sets of moments, may arise with QMOM/CQMOM when high-order spatial discretization schemes are used for transporting the moments of the NDF (Wright, 2007). A set of moments is valid if there exists a NDF resulting in that specific set of moments: in this way the calculated nodes are always in the domain of internal-coordinate space and the weights are always positive. If the inversion algorithm were used with invalid moment sets, unrealizable quadratures would be calculated (because no realizable NDF corresponds to an invalid set), jeopardizing the stability of the simulation. Wright (2007) proposed an iterative algorithm to correct a corrupted set of moments, based on the convexity principle, but this algorithm is only capable to restore the set, not to prevent and solve the corruption problem. Recently Vikas et al. (2011a) introduced a class of high-order numerical schemes, based on the kinetic finite volume schemes, that guarantees the realizability of a set of moments. DQMOM does not exhibit the corruption problem (Marchisio and Fox, 2005), since the resulting moments tracked by the method will always be realizable as long as the weights are non-negative, but, under certain conditions, the method may be unable to calculate properly the moments. In fact, if the moment transport equation is purely hyperbolic (i.e. pure advection of the NDF) or there are spatial discontinuities in the quadrature, the spatial continuity assumption used to derive the method is no more valid and DQMOM fails (Mazzei et al., 2010, 2012). Even if the spatial solution is smooth, problems may arise whenever the moment transport equation contains spatial diffusion terms that are smaller than or comparable with the numerical diffusion that every Finite-Volume scheme (FV) introduces. In fact, in this case the correction proposed by Marchisio and Fox (2005) is difficult to be calculated since the numerical diffusion coefficient cannot be determined accurately. Very recently, Donde et al. (2011a,b,c) suggested a slight modification of the DQMOM formulation that seems to address the aforementioned problems in the case of turbulent reactive flows described by LES models, wherein the turbulent diffusion term is typically small compared to the convection term. In this work, we will formulate this method in a general way (labeled in what follows as DQMOM-Fully Conservative or DQMOM-FC) and explain the reason why this method is successful by comparing it with CQMOM.

Although the methodology discussed in this work has general validity, here we focus on turbulent gas–liquid systems, in which spatial inhomogeneities, bubble collisions and mass transfer play an important role in the determination of the state of the system. In such a system the mass transfer rate strongly depends on the size of the bubbles (mass transfer from small bubbles is faster than for larger ones) and a second internal coordinate related to the bubble composition is needed in addition to bubble size, in order to determine accurately the evolution of the population. The remainder of the paper is the following: Section 2 contains a very short introduction to the multivariate Population Balance Modeling for turbulent gas–liquid systems. In Section 3, the two multivariate solvers CQMOM and DQMOM will be formulated for homogeneous systems and discussed in details. In Section 4, we will introduce the spatial inhomogeneities and the implications for both methods. In Sections 5 and 6 some numerical experiments carried out to compare the two methodologies will be explained and discussed.

2. Population Balance Modeling for gas–liquid systems

A generic turbulent gas–liquid system can be thought of as a dispersion of bubbles, each one characterized by its size L, composition $\boldsymbol{\phi}_{\mathrm{b}}$ and velocity $\mathbf{U}_{\mathrm{b}}$. In this work, we are interested in the description of an isothermal air–water system, in which only oxygen transfers between air and water (i.e., vector $\boldsymbol{\phi}_{\mathrm{b}}$ becomes a scalar quantity ϕ_{b} representing the total number of moles of oxygen in the bubble).

The entire population of bubbles can be described by a smooth and continuous function $\tilde{n}$, called Number Density Function (NDF), differentiable with respect to time, physical space and internal-coordinate space (i.e., the space generated by the considered properties of the population), in such a way that the following quantity:

$$\tilde{n}(L, \phi_{\mathrm{b}}, \mathbf{U}_{\mathrm{b}}; \mathbf{x}, t)\mathrm{d}L\ \mathrm{d}\phi_{\mathrm{b}}\ \mathrm{d}\mathbf{U}_{\mathrm{b}}\ \mathrm{d}\mathbf{x}, \tag{1}$$

represents the expected number of bubbles with size between L and $L + \mathrm{d}L$, composition between ϕ_{b} and $\phi_{\mathrm{b}} + \mathrm{d}\phi_{\mathrm{b}}$, velocity between $\mathbf{U}_{\mathrm{b}}$ and $\mathbf{U}_{\mathrm{b}} + \mathrm{d}\mathbf{U}_{\mathrm{b}}$ contained inside the physical volume $\mathrm{d}\mathbf{x}$.

Referring to the classical theory of population balances (Ramkrishna, 2000; Vikas et al., 2011b), it is possible to write a continuity statement for the NDF. This equation is called Generalized Population Balance Equation (GPBE):