Chemical Engineering Science 101 (2013) 663–673

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Solution of the population balance equation by the direct dual quadrature method of generalized moments ☆

F.P. Santos, J.L. Favero, P.L.C. Lage *

Programa de Engenharia Química COPPE, Universidade Federal do Rio de Janeiro, PO Box 68502, Rio de Janeiro, RJ 21941-972, Brazil

HIGHLIGHTS

- The direct DuQMoGeM is introduced for the solution of population balance problems.
- As DQMOM, this method also solves for the quadrature abscissas and weights.
- Differently from DQMOM, the direct DuQMoGeM is a dual-quadrature method.
- The quadrature errors in direct DuQMoGeM can be controlled by an adaptive cubature.
- Both methods were compared for problems with breakage, aggregation and growth.

ARTICLE INFO

Article history:
Received 7 December 2012
Received in revised form
4 March 2013
Accepted 15 July 2013
Available online 24 July 2013

Keywords:
Population balance
Numerical methods
Direct Quadrature Methods of Moments
Generalized moments
Multiphase flow
Particulate systems

ABSTRACT

The Direct Dual Quadrature Method of Generalized Moments (D^2uQMoGeM) was formulated for the solution of the population balance equation. It mixes the properties of the Direct Quadrature Method of Moments (DQMoM) and the Dual Quadrature Method of Generalized Moments (DuQMoGeM). The weights and weighted abscissas are tracking directly as in DQMoM and the quadrature errors are controlled by an adaptive quadrature as in DuQMoGeM. The D^2uQMoGeM was implemented and tested for several different problems with analytical solutions. It was shown to be more accurate than DQMoM with a reasonable increase in computational time.

1. Introduction

Polydisperse multiphase flows are present in several industry processes. These flows can be modeled by a mesoscopic approach called Population Balance (PB) combined with the Eulerian multi-fluid flow formulation (Silva and Lage, 2011), which may be called PB-CFD simulations. The population balance equation (PBE) is the conservation equation for the number of particles, represented by the mean number density function, which depends on the particle properties, the physical space and time (Ramkrishna, 2000). This mesoscopic framework has a large range of applicability and there is a considerable impetus for the development of numerical methods for solving the PBE (Bove et al., 2005; Strumendo and Arastoopour, 2008; Fox et al., 2008; Massot et al., 2010; Attarakih et al., 2009; Lage, 2011; Yuan et al., 2012, among others). Despite these efforts, there is still a lack of accurate and robust techniques for analyzing the dynamics of particle systems.

Basically, there exist four classes of well established methods to solve the PBE: Monte-Carlo methods, discretization methods, moment methods closed by quadrature and weighted residual methods. In the following, we focused on the quadrature-based moment methods (QBMM) and their variants.

The first QBMM was the quadrature method of moments (QMoM). The QMoM solves the moments of the number density function (NDF) and the integral terms of the PBE are approximated by an N-point Gauss–Christoffel quadrature rule, that is, a Gaussian quadrature whose weight function is the particle number density function (McGraw, 1997). In this method, the N-point Gauss–Christoffel needs to be calculated from the first $2N$ moments using the Product-Difference algorithm (PDA) (Gordon, 1968) or the Modified Chebyshev method (MCM) (Wheeler, 1974).

☆This article is dedicated to Professor Alberto Luiz Coimbra, in the 50th anniversary of COPPE (1963–2013), the Graduate School of Engineering of the Federal University of Rio de Janeiro.

* Corresponding author. Tel.: +55 21 2562 8346; fax: +55 21 25628300.
E-mail addresses: paulo.lage@gmail.com, paulo@peq.coppe.ufrj.br (P.L.C. Lage).
URL: http://www.peq.coppe.ufrj.br/pesquisa/tfd (P.L.C. Lage).

0009-2509/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ces.2013.07.025

Afterwards, Marchisio and Fox (2005) developed the Direct QMoM (DQMoM), in which the weights and abscissas are tracked in time and space instead of the moments of the NDF. Therefore, DQMoM solves the PBE without calculating the Gauss–Christoffel quadrature during the solution, which reduces the computational cost. The Gauss–Christoffel quadrature provides a discretization in the internal variable, which yields N particle phases in an Eulerian multifluid approach for polydispersed multiphase flows, being the reason why these methods are considered well-suited for PB-CFD simulations (Silva and Lage, 2011).

Nonetheless, QMoM and DQMoM have some limitations. Both are unable to reconstruct the distribution function, whose values must be calculated at the lower boundary of the particle size space for some problems with a negative growth rate (Massot et al., 2010). Furthermore, the N-point Gauss–Christoffel calculation is an ill-conditioned problem what may limit the number of quadrature points that can be used in the QBMM (Gautschi, 2004). Since the number of quadrature points also controls the QBMM accuracy, a small number of quadrature points are not usually enough to represent the integral terms of the integrated PBE (Dorao and Jakobsen, 2006a, b). Hence, this might yield a poor representation of the physical behavior of the moments and even a loss of the positiveness of the measure defined by them (Petitti et al., 2010).

Several variants of QMoM and DQMoM have been developed. In the following, these variants are shortly reviewed.

Alopaeus et al. (2006) proposed the usage of fixed-point quadrature rules (FQMoM). This approach avoids some robustness and accuracy problems associated to the Gauss–Christoffel quadrature computation. By analyzing several problems, they concluded that FQMoM was better than QMoM in accuracy and computational cost.

Grosch et al. (2006) solved the moment equations and the quadrature moment approximation simultaneously as a differential algebraic system of equations (DAE). However, they did not obtain a significant improvement compared to the standard QMoM. Nagy et al. (2009) applied a similar methodology for several mechanisms using an analytical Jacobian matrix in the DAE system. The authors observed an enhancement of robustness and accuracy for pure growth problems but not for cases with breakage and aggregation. This occurs due to the intrinsic quadrature errors of QMoM. Later on, Nagy et al. (2012) used automatic differentiation (AD) to compute the Jacobian matrix of the DAE-QMoM. This method, termed AD-QMoM, was more robust and at least 2 times faster than DAE-QMoM for the same level of accuracy. Nevertheless, it still presents the intrinsic quadrature error of QMoM.

Su et al. (2007) proposed the usage of an adjustable factor, s, in QMoM, whose purpose is to improve the robustness in the the Gauss–Christoffel quadrature calculation. Basically, they used fractional moments given by

$$\mu_{k/s} = \int_0^\infty x^{k/s} f(x,t)\,dx = \sum_{\alpha=1}^{N} x_\alpha^{k/s}\omega_\alpha \tag{1}$$

and defined $\tilde{x} = x^{1/s}$ as equivalent abscissas which were then calculated by the product-difference algorithm (Gordon, 1968).

Afterwards, Su et al. (2008) applied the same idea to DQMoM but using an adaptive procedure to chose the value of the adjustable factor, calling the method as Adaptive DQMoM (ADQMOM). The value of the adjustable factor was determined by a search procedure based on the conditional number of the ADQMoM system of linear equations.

Attarakih et al. (2009) proposed the sectional QMoM (SQMoM), focusing on reconstructing the NDF. The domain is divided into sections whose sectional moments are then used to determine a quadrature for each section, as in QMoM. Although the Gauss–Christoffel quadrature was also used, Attarakih et al. (2009) recommended an equal-weight two-point quadrature with better numerical properties.

Qamar et al. (2011) applied QMoM for solving a univariate PBE using the moments of polynomials to compute the Gauss–Christoffel quadrature for closure. These polynomials are orthogonal in relation to the measure defined by the particle number distribution function and their generalized moments were used to obtain the coefficients in the three-term recurrence relation and then the quadrature points. They stated that this determination of the quadrature rule avoids the ill-conditioned issue present in PDA and MCM (John & Thein, 2012). However, they applied the method with just three quadrature points which usually does not lead to an ill-conditioned problem. In essence, the quadrature rule computation is similar to that used in DuQMoGeM (Lage, 2011), where the modified Chebyshev method was applied to the generalized moments of known families of orthogonal polynomials (for instance Legendre, Laguerre) to compute the coefficients in the recurrence relation. However, the later procedure is better conditioned (Gautschi, 1994). Later on, the method extension for bivariate population balance equation was proposed by Qamar et al. (2010), using an arbitrary transformation of the two internal variables into the independent variable of the polynomials. This method leads to a three-point quadrature whose determination involves a specific set of generalized mixed moments with orders as large as ten.

Massot et al. (2010) introduced a modified sectional DQMoM combined with the method of characteristics. Since they were interested in droplet evaporation problems, the entropy maximization (EM) reconstruction technique was used to rebuild the NDF in order to evaluate the particle flux at the lower boundary of the particle size space. They simulated some evaporation problems, showing that the modified sectional DQMoM is accurate and stable for describing the dynamics of the moments. However, the EM numerical complexity increases significantly when it is applied to a multi-dimensional NDF (Yuan et al., 2012).

An interesting technique that is able to reconstruct the NDF from a finite number of its moments is the kernel density element method (KDEM) (Athanassoulis and Gavriliadis, 2002). The KDEM expresses the NDF in terms of the superposition of Kernel Density Functions (KDF), which has special features that can ensure the positivity of the reconstructed NDF. In essence, this method is similar to EM. It also uses functions (KDF) whose unknown parameters are obtained by solving a minimization problem based on the moments of the NDF. Based on this idea, Yuan et al. (2012) developed a method called EQMoM, which mixes the properties of QMoM and KDEM. EQMoM is a dual-Gaussian quadrature method which uses a unique parameter to determine the KDFs, which is obtained from an additional moment equation. The results obtained by Yuan et al. (2012) were very good for all studied cases.

As it has already been cited, the QBMM usually suffers from error accumulation due to the quadrature approximations, which can eventually degenerate the PBE solution. In order to overcome this inherent problem, Lage (2011) developed the Dual Quadrature Method of Generalized Moments (DuQMoGeM). In this method, the quadrature errors can be controlled using adaptive numerical integration (Favero and Lage, 2012). For this reason, DuQMoGeM attained better results than QMoM for all cases studied by Lage (2011). However, this methodology has some shortcomings. It also tracks the moments of the distribution and, therefore, cannot be used to simulate a polydisperse multiphase flow when the particle velocity depends on the internal variables.

In this work, the Direct Dual Quadrature Method of Generalized Moments (D^2uQMoGeM) was formulated and tested. D^2uQMoGeM uses the same idea behind DQMoM to make DuQMoGeM a direct method. The weights and weighted abscissas are tracking directly as in DQMoM and the quadrature errors are controlled by an