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Solution of the Population Balance Equation using the Sectional Quadrature Method of Moments (SQMOM)

Menwer M. Attarakih[a], Hans-Jörg Bart[b,] and Naim M. Faqir[c]*

[a]*Al-Balqa Applied University, Faculty of Engineering Tech., Chem. Eng. Dept., PO.Box 15008, 11134-Amman, Jordan.*

[b] *University of Kaiserslautern, Faculty of Mechanical & Process Engng., Institute of Process Engng., POB 3049, D-67653 Kaiserslautern, Germany*

[c]*Naim M. Faqir, University of Jordan, Faculty of Engng. & Technology, Chemical Engng. Department, 11942 Amman, Jordan*

**Corresponding author: E-mail: bart@mv.uni-kl.de, http://www.uni-kl.de/LS-Bart/*

Abstract

A numerical framework is introduced for solving the population balance equation based on accurately conserving (from theoretical point of view) an unlimited number of moments associated with the particle size distribution. The key idea in this work is based on the concept of primary and secondary particles, where the former is responsible for the distribution reconstruction while the latter one is responsible for different particle interactions such as breakage and coalescence. The numerical method is found to assemble all the advantages and disadvantages of the sectional and moment methods and hence the name: SQMOM. The method is illustrated here by considering pure breakage in a well-stirred vessel; however, it is already extended and tested for particle coalescence (agglomeration) and growth.

Keywords: population balance, SQMOM, sectional methods.

1. Introduction

Population balance equation (PBE) forms nowadays the cornerstone for modeling dispersed-phase systems arising in many engineering applications such as aerosols dynamics, crystallization, precipitation, liquid-liquid, gas-liquid and combustion processes. The resulting model equations of these processes range from integro-differential to integro-partial differential equations with no general analytical solutions. Accordingly, there exist in the literature many numerical methods as attempts to solve certain type of the PBEs. These methods ranges from simple finite differences (FDS) or sectional methods using linear grids (in terms of particle diameters) to Galerkin and orthogonal collocations methods on finite elements. An exhaustive review of the available numerical methods is presented by Attarakih et al. (2004a). The quadrature method of moments (QMOM) as first introduced by McGraw (1997) to solve the PBE with pure growth is found very efficient from accuracy and computational cost point of view. Unlike the sectional (finite difference) methods, the QMOM has a drawback of destroying the shape of the distribution and retain information about it only through information stored in its moments. A recent comparison between the QMOM and the finite difference schemes could be found in Attarakih et al. (2006). On the other hand, one limitation of the finite difference schemes is their inability to predict accurately

integral quantities (low-order moments as a especial case) associated with populations of sharp shapes (Ramakrishna, 2000).
So, the objective of this work is whether it is possible to have a finite difference scheme that retains the advantages of the QMOM without destroying the shape of the distribution? The answer to this question is yes, where it is found in this work that all the attempts made previously to increase the accuracy of the finite difference schemes such as the fixed and moving pivot techniques (Ramkrishna, 2000) or the conservative descretization approach of the present authors (Attarakih et al., 2004b) are all merely limited answers to the above question. In this work the fundamental framework to combine the FDS and the QMOM is introduced and thoroughly tested using the available analytical solutions when it is possible. It is found that the new framework as it is called the Sectional Quadrature Method Of Moments (SQMOM) is very accurate in solving the PBEs and furnish a Gauss-like quadrature to evaluate any integral quantity associated with the population density.

2. The Population Balance Equation

The population balance equation for a well-stirred continuous vessel of residence time, τ, could be written as:

$$\frac{\partial f(d,t)}{\partial t} = \frac{f^{feed} - f}{\tau} - \Gamma(d) f(d,t) + \int_d^{d_{\max}} \Gamma(d')\beta(d \mid d') f(d') \partial d' \qquad (1)$$

where *f(d,t)* is the average number of droplets per unit volume of the vessel at time *t*. The first term on the left hand side denotes the rate of accumulation of droplets of size *d*. The term on the right hand side is the net rate of particles as a result of entry and exit events, breakage and coalescence. The source term, is rather complex and for simplicity, only the breakage part is presented (for the complete details see Ramkrishna, 2000). Γ and β are the breakage frequency and the daughter particle distribution respectively.

3. The Sectional Quadrature Method Of Moments (SQMOM)

In the finite difference or sectional methods the particle size (here is denoted by the particle diameter, *d*) is discretized into finite number of sections, M_s. The population in each section is considered to behave like a single particle, and hence it is concentrated at a representative size usually at the middle of the section. In the present framework of descretization, this single particle will be called the primary particle and it will be responsible for the reconstruction of the shape of the distribution. In this way, the greater the number of primary particles (M_s), the more accurate is the reconstruction of the distribution. Unfortunately, large number of primary particles is required to estimate integral quantities of the distribution accurately and hence increasing extensively the computational loads when the population balance equation is coupled for example to a CFD calculations (Marchisio and Fox, 2005). The interaction between primary particles in different sections, due to breakage event for example, results in a new primary particle with no representative size due to the discrete approximation of the distribution. Because of the newly-birthed particle could not conserve any of its low order moments but one (if it is located at the middle of the section), the rest of the low-order moments are predicted with low accuracy and hence the associated integral quantities.

To overcome this fundamental problem of the sectional methods, secondary particles are generated in each section with positions (abscissas) $d_j^{<i>}, i=1,2,...M_s, j=1,2,...N_q$ (see Fig.(1) upper panel), where the number of these secondary particles dictates the desired number of low-order moments to be conserved. The population density in each section is partitioned between these particles according to the variation of the population density in this section by assigning weights ($w_j^{<i>}, i=1,2..M_s, j=1,2..N_q$) to each particle. These secondary particles are exactly equivalent to the number of quadrature points in Gauss-like quadratures or the QMOM. Accordingly, each secondary particle could conserve or reproduce two low-order moments and in general $2N_q$ moments, where N_q is the number of secondary particles.

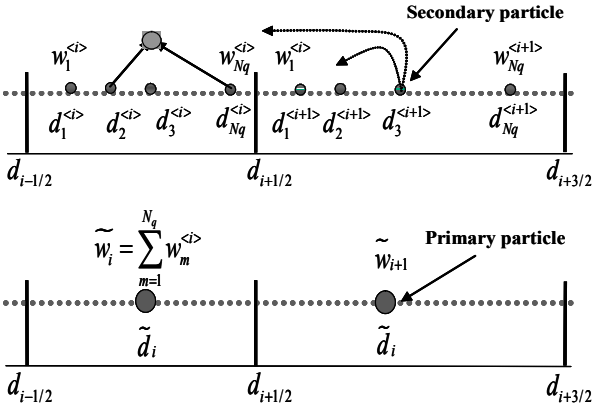

Fig.(1): The concept of primary and secondary particles.

In this framework, the particle mechanisms such as breakage and coalescence occur through interactions between the secondary particles. It is obvious from Fig.(1) above (the upper panel) that $N_q \times M_s$ particles are contributing in the breakage and coalescence events. The distribution could be reconstructed from the secondary particles by averaging the total weights of the secondary particles with respect to the section width and locating it at the mean size of the secondary particles as shown in Fig.(1) (the lower panel). In pure mathematical sense, the above presentation is equivalent to applying the QMOM to each section of arbitrary width: $[d_{i-1/2}, d_{i+1/2}]$, $i=1,2,...M_s$ resulting in a set of sectional moments that could be written as:

$$\mu_r^{<i>}(t) = \int_{d_{i-1/2}}^{d_{i+1/2}} d^r f(d,t) \partial d, \qquad r = 0,1,2...2N_q - 1 \tag{2}$$

By applying this set of moment transformations to Eqs.(1) and after some algebraic manipulations one could get:

$$\frac{d\mu_r^{<i>}(t)}{dt} = \frac{\mu_r^{<i>,feed} - \mu_r^{<i>}}{\tau} - B_r^{<i>}\left[\Gamma^{<i>} \bullet w^{<i>}\right]^T + \sum_{m=i}^{M_s} C_r^{<i,m>}\left[\Gamma^{<i>} \bullet w^{<i>}\right]^T \tag{3}$$

where:

$$B_r^{<i>} = \left[(d_1^{<i>})^r \quad (d_2^{<i>})^r \quad .... \quad (d_{N_q}^{<i>})^r \right],$$

$$\Gamma^{<i>} = \left[\Gamma(d_1^{<i>}) \quad \Gamma(d_2^{<i>}) \quad .... \quad \Gamma(d_{N_q}^{<i>}) \right], w^{<i>} = \left[w_1^{<i>} \quad w_2^{<i>} \quad .... \quad w_{N_q}^{<i>} \right] \text{and,}$$

$$C_r^{<i,m>} = \left[\int_{d_{i-1/2}}^{\min(d_{i+1/2}, d_1^{<m>})} d^r \beta(d \mid d_1^{<m>}) \partial d \quad ... \quad \int_{d_{i-1/2}}^{\min(d_{i+1/2}, d_{N_q}^{<m>})} d^r \beta(d \mid d_{N_q}^{<m>}) \partial d \right]$$

Note that each secondary particle in the *i*th section is characterized by its location (abscissa), $d_j^{<i>}$, and weight, $w_j^{<i>}$. These characterization variables are only function of time and could be calculated by inverting the *i*th moment problem assuming equal number of secondary particles in each section as follows:

$$\mu_r^{<i>} = \sum_{j=1}^{N_q} (d_j^{<i>})^r w_j^{<i>} \tag{4}$$

The above $2N_q$ equations are solved uniquely for the N_q abscissas and N_q weights using the standard product-difference algorithm as outlined by McGraw (1997). For the special cases of one and two secondary particles an analytical solution could be found. The solution when one secondary particle is used is trivial; however, for two secondary particles ($N_q = 2$) the algebraic manipulations are rather involved (but straight forward) and the result is presented below:

$$d_{1,2}^{<i>} = \frac{1}{2}\psi(\mu_{r,r=0,1,2,3}^{<i>}) \pm \frac{1}{2}\sqrt{\psi^2(\mu_{r,r=0,1,2,3}^{<i>}) - 4\chi(\mu_{r,r=0,1,2,3}^{<i>})} \tag{5}$$

$$w_{1,2}^{<i>} = \mu_0^{<i>} \left(\frac{\sigma}{\tilde{d} - d_{1,2}} \right)_{<i>}^2 \frac{1}{1 + \left[\sigma / [\tilde{d} - d_{1,2}] \right]_{<i>}^2} \tag{6}$$

where: ψ, χ, σ are functions of the first four moments and $\tilde{d}^{<i>} = \mu_1^{<i>} / \mu_0^{<i>}$

The system given by Eqs(3), (5) and (6) is a differential algebraic equation system (DAE) that could be reduced to only a differential system by substituting Eqs.(5) and (6) into (3). Note that it is clear by this combination that the solution of the system (3) guarantees the conservation (reproduction) of $2N_q$ low order moments ($\mu_{r,r=0,1,...2N_q-1}$). Since the number of secondary particles, N_q, is unlimited from theoretical point of view, it follows that the discretized PBE given by the system (3) is guaranteed to reproduce an unlimited number of low-order moments (internally consistent with respect to $2N_q$ moments). This makes the present framework of discretization generally consistent and accurate for solving general PBEs without placing any assumption on the shape and type of the distribution or breakage functions. Accordingly, all the attempts in the literature that are concerned with conserving certain and hence limited number of moments appear to be special cases of the present descretization method by varying the number of primary and secondary particles. For example, when the number of the primary particles equals one the standard QMOM is recovered, while when the number of secondary particles equals one, the standard moving pivot technique is recovered by conserving the total number and volume of the particles in each section (the zero and third moments are conserved).

4. Numerical Results and Discussion

Due to the space limitation, only one example is presented here for the case of particle (droplet) breakage in a well-mixed continuous vessel where the analytical solution for Eq.(1) is available (Attarakih et al., 2004b) using the following set of functions: $f^{feed} = 3d^2 e^{-d^3}$, $\Gamma = d^6$, $\beta = 6d^2 / d'^3$, $f(d,0) = 0$, $d_{\min} = 0.001$, $d_{\max} = 2$ and $\tau = 100s$. The sectional moments are evolved in time using the trapezoidal rule with fixed step size of 0.1 second. First, Fig.(2a) compares the convergence of the SQMOM at fixed number of secondary particles by varying the number of primary particles from 2 to 4. It is clear how the first two moments (μ_0 & μ_1) are over predicted using only two primary and secondary particles. The inaccuracy is attributed to the sharpness of the distribution as it is evolved in time (see Fig. 3a). By doubling the number of primary particles or equivalently the number of sections, the width of each section is decreased resulting in an accurate integration over the sharp distribution as expected where this fact is true for all Gauss-like quadrature methods. On the other hand, by increasing the number of secondary particles from 2 to 3 as seen in Fig.(2b), the same result is almost obtained, which is expected since the accuracy of the quadrature methods is increased by increasing the number of the quadrature points (secondary particles).

In Fig.(3a), the average number concentration as predicted using the SQMOM is compared to the analytical solution at different periods of time. It is clear that using 35 primary particles is enough to follow the shape of the number concentration function very accurately. However, since the predicted shape of the distribution is not used in the prediction of any integral property, small number of primary particles is found enough to get an idea about the shape of the distribution. Consequently, the location and weights (Eqs.(5) & (6)) of the secondary particles is used to evaluate any integral over the unknown distribution with the desired accu racy.

To get more insight on the convergence properties of the SQMOM, the systematic error ($d30^{anal.} - d30^{num.}$) based on the mean particle diameter ($d30 = \mu_3 / \mu_0$) is studied as function of the number of primary and secondary particles. It is evident that the order of convergence is increased by increasing both the primary and secondary particles due to the increasing accuracy of evaluating the unclosed integrals in the PBE. The increasing accuracy by increasing the number of secondary particles is reported by many researchers (McGraw, 1997 and Marchisio, 2005).

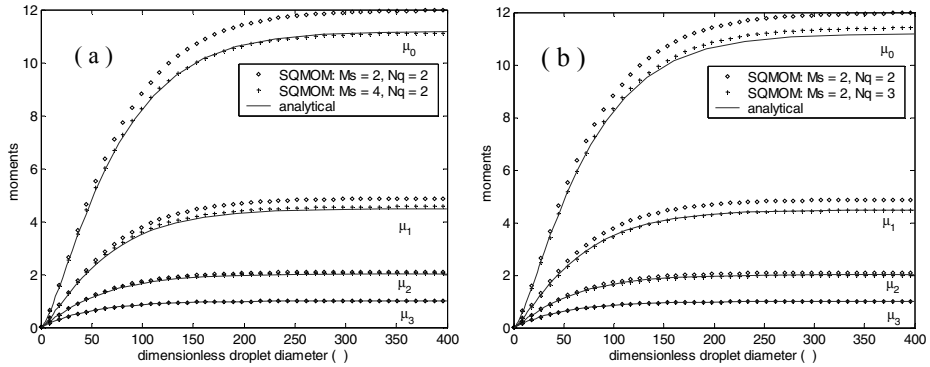

Fig.(2): Convergence of the first four moments using the SQMOM: a- By varying the number of primary particles. b- By varying the number of secondary particles.

The present framework is already extended to particle coalescence and growth where the results are found very accurate and the computational load is dependent on the accuracy and details needed by the user.

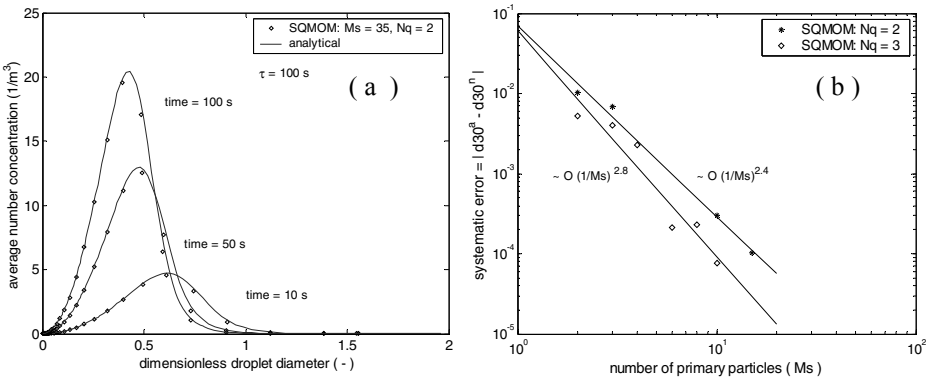

Fig.(3): a- Comparison between the analytical solution and that predicted by the SQMOM. b – Convergence of the SQMOM in terms of the systematic error in *d30*.

5. Conclusions

The present framework for solving the PBE based on the concept of the primary and secondary particles is found general where all the previous attempts in literature to overcome the problem of internal consistency are merely especial cases of the present framework. In this way, the primary particles are responsible for the distribution reconstruction, while the secondary ones are responsible for breakage, coalescence .. etc. events and carry a lot of information about the distribution. The SQMOM is found extremely accurate and converges very fast by increasing either the number of primary or secondary particles; however, at the expense of the computational load. This computational load is up to the user and the degree of details required about the distribution. Accordingly, the flexibility of the method by its reduction to the standard QMOM when the number of primary particles equals one makes it very attractive from computational point of view. For example, if if $M_s = 1$ and $N_q = 2$, only four ODEs are to be solved; however, if $M_s = 5$ and $N_q = 2$, then twenty ODEs are to be solved.

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