World Applied Sciences Journal 23 (12): 41-47, 2013
ISSN 1818-4952

DOI: 10.5829/idosi.wasj.2013.23.12.416

Bivariate Extension of Quadrature Method of Moments for Solving Volume-Based Population Balance Models

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Abstract: This paper presents a bivariate extension of Quadrature Method of Moments (QMOM) for the solution of dynamic volume-based two-dimensional Population Balance Models (PBMs) involving kinetic processes of nucleation, size dependent growth and aggregation. The method is based on orthogonal polynomials for calculating pairs of quadrature abscissas (points) and weights. For better accuracy of the method, a third order orthogonal polynomial is chosen to calculate the quadrature points and weights. Two numerical test problems are discussed. For validation, the numerical results are compared with analytical solutions. In both the problem, the proposed method was found to be efficient and accurate.

Key words: Particulate processes . volume-based two-dimensional population balance model . quadrature method of moments . orthogonal polynomials

INTRODUCTION

The Population Balance Models (PBMs) have been used for model the variety of particulate systems. These models form hyperbolic partial differential equations and simulate a wide range of particulate processes including comminution, crystallization, granulation, flocculation, combustion and polymerization. The major phenomena that influence these processes include growth, nucleation, aggregation, breakage, dissolution and inlet and outlet streams. Analytical solutions to the PBM can only be obtained for very few special cases. Therefore, numerical techniques played an important role to approximate these problems for the last three decades. Different solution techniques are available in the literature to solve certain type of PBE, Hulburt and Katz [1], Barrett and Jheeta [3], Marchisio *et al*. [4], McGraw [5], Lim *et al*. [6], Rawlings *et al*. [7], Rosner *et al*. [8], Tandon and Rosner [9], Qamar *et al*. [10, 11]. However, a majority of the numerical methods for bivariate PBEs in the open literature require further testing, especially for combined processes at long simulation times.

The Quadrature Method of Moments (QMOMs), initially introduced by McGraw [5] for solving PBE with pure growth term, was found to be very efficient from computational cost point of view. The mth order moment is defined by integrating the population number density function with respect to certain property variable (e.g. particle sizes, particle volumes) weighted with this property raised to its mth power. The lower order moments contain important information about the particle size distribution (e.g. number and total volume of particles). However, this approach often leads to an unclosed set of moment equations Hulburt and Katz [1], Ramkrishna [12]. In this method, quadrature approximation was used for solving integrals of PSD and the required abscissas and weights were obtained by using the Product Difference (PD) algorithm of Gordon [13]. Further work in this direction can be found in (Fan *et al*. [14], Lage [15], Marchisio *et al*. [4, 16], McGraw [17] and Qamar *et al*. [18]). Most of this published work is associated with only one property coordinate. However, Wright *et al*. [19] were among the first who tried to extend this method to bivariate PBEs to simulate inorganic nano-particles undergoing simultaneous co-agulation and sintering. The QMOM are famous for their low computational cost and good accuracy.

These methods are useful when the knowledge of size-distribution is not directly needed and the lower-order moments are sufficient to recover the important

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quantities, for example evolution of aerosol and clouds McGraw [17]. Moreover, QMOM are suitable when PBM is combined with CFD code, see for example McGraw [17], Marchisio *et al*. [16].

In the present work, a different approach is used to derive QMOM for solving volume-based bivariate PBMs incorporating particles nucleation, size dependent growth and aggregation phenomena. The proposed method is based on orthogonal polynomials for calculating the quadrature abscissas and corresponding weights, see Press *et al*. [20]. Here, a third order polynomial is chosen, which requires 36-moments for bivariate PBM to calculate pairs of quadrature points and weights. However, the method has no restriction on the number of moments for any chosen polynomial, the required number of moments increases as the order of polynomial increases. Two numerical test problems are considered. The numerical results of QMOM are validated against the analytical solutions.

This article is arranged as follows. In section 2, the mathematical model of bivariate volume-based PBE is introduced. In section 3, the proposed bivariate extension of QMOM is derived for PBEs. In section 4, numerical test problems are carried out. Finally, section 5 offers conclusions and remarks.

BIVARIATE POPULATION BALANCE EQUATION

In this section, a mathematical model for ideally mixed volume-based bivariate population balance equation is introduced. A population of particles is characterized by its Particle Size Distribution (PSD) which is mathematically described by a number density function n(t; x; y) as a function of time t and volumes-coordinates (x; y). The general volume-based bivariate PBE for a particulate system undergoing growth, nucleation and aggregation is given as (Hulburt and Katz [1], Randolph and Larson [2])

$$\begin{aligned}\frac{\partial n(t,x,y)}{\partial t} = & -\underbrace{\frac{\partial[G_1(t,x)n(t,x,y)]}{\partial x}}_{\text{growth along x-axis}} - \underbrace{\frac{\partial[G_2(t,y)n(t,x,y)]}{\partial y}}_{\text{growth along y-axis}} + \underbrace{D_{nuc}}_{\text{nucleation}} \\ & + \underbrace{\frac{1}{2}\int_0^x\int_0^y \beta(t,x-x',y-y',x',y')\,n(t,x-x',y-y')\,n(t,x',y')\,dx'dy'}_{\text{birth due to aggregation}} \\ & - \underbrace{\int_0^\infty\int_0^\infty \beta(t,x,y,x',y')\,n(t,x',y')\,n(t,x,y)\,dx'dy'}_{\text{death due to aggregation}}\end{aligned} \tag{1}$$

The klth moment $m_{k,l}(t)$ of this number density n(t,x,y) is defined as

$$m_{k,l}(t) = \int_0^\infty\int_0^\infty x^k y^l n(t,x,y)\,dx\,dy \tag{2}$$

After applying the above moments transformation, the PBE (1) gives

$$\begin{aligned}\frac{dm_{k,l}(t)}{dt} = & \underbrace{\int_0^\infty\int_0^\infty kx^{k-1}y^l G_1(t,x)n(t,x,y) + lx^k y^{l-1} G_2(t,y)n(t,x,y)\,dx\,dy}_{\text{growth}} + \underbrace{\int_0^\infty\int_0^\infty x^k y^l D_{nuc}\,dx\,dy}_{\text{nucleation}} \\ & + \underbrace{\frac{1}{2}\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty \beta(t,u,v,x',y')(u+x')^k(v+y')^l n(t,u,v)\,n(t,x',y')\,dx'dy'du\,dv}_{\text{birth due to aggregation}} \\ & - \underbrace{\int_0^\infty\int_0^\infty y^l x^k n(t,x,y)\int_0^\infty\int_0^\infty \beta(t,x,y,x',y')\,n(t,x',y')\,dx'dy'dx\,dy}_{\text{death due to aggregation}}\end{aligned} \tag{3}$$

The standard quadrature method is not able to solve the above integrals due to volume-dependent growth rate and due to complicated integrands of the bivariate aggregation term. However, Quadrature method of moments can be applied to solve the complication which is explained in Section 3.

THE QUADRTURE METHOD OF MOMENTS FOR BIVARIATE PBE

At this part of the manuscript, we discuss the QMOM for solving different integrals appearing in the bivariate PBE. Consider an integral of the form $\int_a^b\int_c^d \psi(x,y)g(x,y)dxdy$, where $\psi(x,y)$ is a non-negative weight function and g(x,y) is a non-specified function of x and y, then the Gaussian quadrature method approximates the integrals in (3) in the given domain as

$$\int_a^b\int_c^d \psi(x,y)g(x,y)dxdy \approx \sum_{j=1}^{N} w_j g(x_j, y_j) \tag{4}$$

The orthogonal polynomials are used to find weight w_j and abscissa (x_j,y_j). Let us define the scalar product of two functions r(x,y) and s(x,y) over a weight function $\psi(x,y)$ as:

$$< r \backslash s >= \int_a^b\int_c^d \psi(x,y)r(x,y)s(x,y)dxdy \tag{5}$$

The functions r(x,y) and s(x,y) are said to be orthogonal if their scalar product is zero. In this case moments of PSD are approximated as

$$m_{k,l}(t) = \int_0^\infty\int_0^\infty x^k y^l n(t,x,y)dxdy \approx \sum_{j=1}^{N} x_j^k y_j^l w_j \tag{6}$$

where, n(t,x,y) plays a role of weight function $\psi(x,y)$ and x_j and y_j are the quadrature points. In this study, we choose N = 3. After applying the quadrature rule (6), the integral terms in (3) can be approximated as

$$\begin{aligned}\frac{dm_{k,l}(t)}{dt} &= k\sum_{i=1}^{N}(x_i)^{k-1}y_i^l w_i G_1(t, x_i)\\ &+ l\sum_{i=1}^{N}(x_i)^k y_i^{l-1} w_i G_{21}(t, y_i) + d_{nuc}^{(kl)}\\ &+ \frac{1}{2}\sum_{i=1}^{N} w_i \sum_{j=1}^{N}(x_i + x_j)^k (y_i + y_j)^l \beta(t, x_i, y_i, x_j, y_j) w_j\\ &- \sum_{i=1}^{N}\sum_{j=1}^{N}(x_i)^k (y_i)^l w_i \beta(x_i, y_i, x_j, y_j) w_j \quad k, l = 0,1,2,....\end{aligned} \tag{7}$$

where

$$d_{nuc}^{(kl)} = \int_0^\infty\int_0^\infty x^k y^l D_{nuc} dxdy$$

Let us consider the recursion relation as given in Safyan *et al*. [21] and simply replace x by x + xy + y = z(x, y). Then the following relation can be obtained,

$$p_{-1} = 0,\ p_0 = 1,\ p_j = (z - a_j)p_{j-1} - b_j p_{j-1},\ j = 1,2,.... \tag{8}$$

with

$$a_j = \frac{< zp_{j-1} / p_{j-1} >}{< p_{j-1} / p_{j-1} >},\ j = 1,2,.... \tag{9}$$

$$b_j = \frac{< p_{j-1} / p_{j-1} >}{< p_{j-2} / p_{j-2} >},\ j = 2,3,.... \tag{10}$$

Since n(t,x,y) is used as weight function $\psi(x,y)$, therefore Eq. (5) becomes

$$< p_j / p_j >= \int_a^b\int_c^d n(t,x,y)p_j^2 dxdy$$

From Eq. (8), the firrst order polynomial can be calculated as,

$$p_1(z) = (z - a_1)\,p_0 = (z - a_1)$$

Here, a_1 is needed to specify p_1. This is given as

$$a_1 = \frac{< zp_0 / p_0 >}{< p_0 / p_0 >} = \frac{\int_0^\infty\int_0^\infty (x + xy + y)n(t,x,y)p_0^2 dxdy}{\int_0^\infty\int_0^\infty n(t,x,y)p_0^2 dxdy} = \frac{m_{1,0} + m_{1,1} + m_{0,1}}{m_{0,0}}$$

Thus, we have

$$p_1(z) = z - \frac{\tilde{m}_{1,1}}{m_{0,0}} \tag{11}$$

where

$$\tilde{m}_{1,1} = m_{1,0} + m_{1,1} + m_{0,1} \tag{12}$$

Next, p_2 can be defined as

$$p_2(z) = (z - a_2)p_1 - b_2 p_0 \tag{13}$$

where according to (9) an (10)

$$a_2 = \frac{< zp_1 / p_1 >}{< p_1 / p_1 >} = \frac{\int_0^\infty\int_0^\infty zn(t,x,y)p_1^2 dxdy}{\int_0^\infty\int_0^\infty n(t,x,y)p_1^2 dxdy} = \frac{\tilde{m}_{3,3}m_{0,0}^2 - 2m_{0,0}\tilde{m}_{1,1}\tilde{m}_{2,2} + \tilde{m}_{1,1}^3}{\tilde{m}_{2,2}m_{0,0}^2 - m_{0,0}\tilde{m}_{1,1}^2} \tag{14}$$

Here, $\tilde{m}_{1,1}$ is given by Eq. (12) and

$$\tilde{m}_{2,2} = m_{2,0} + m_{0,2} + 2(m_{2,1} + m_{1,2} + m_{1,1}) + m_{2,2} \tag{15}$$

$$\tilde{m}_{3,3} = m_{3,0} + m_{0,3} + 3(m_{3,1} + m_{1,3} + m_{2,1} + m_{1,2} + m_{3,2} + m_{2,3} + 2m_{2,2}) + m_{3,3} \tag{16}$$

Similarly Eqs. (10) and (11) gives

$$b_2 = \frac{<p_1/p_1>}{<p_0/p_0>} = \frac{\int_0^\infty\int_0^\infty zn(t,x,y)\left(z - \frac{\tilde{m}_{1,1}}{m_0}\right)^2 dxdy}{\int_0^\infty\int_0^\infty n(t,x,y)dxdy} = \frac{\tilde{m}_{2,2}m_{0,0} - \tilde{m}_{1,1}^2}{m_{0,0}^2}$$

Hence, Eq. (13) for the second order polynomial becomes

$$p_2(z) = \frac{z^2(m_{0,0}\tilde{m}_{2,2} - \tilde{m}_{1,1}^2) + z(\tilde{m}_{1,1}\tilde{m}_{2,2} - m_{0,0}\tilde{m}_{3,3}) + \tilde{m}_{1,1}\tilde{m}_{3,3} - \tilde{m}_{2,2}^2}{m_{0,0}\tilde{m}_{2,2} - \tilde{m}_{1,1}^2} \tag{17}$$

In this manner, one can calculate polynomials of higher order. The third order polynomial $p_3(z)$ is given as

$$p_3(z) = (z)^3 + \eta_2(z)^2 + \eta_1(z) + \eta_0 \tag{18}$$

Where

$$\eta_2 = \frac{\tilde{m}_{2,2}\tilde{m}_{4,4}\tilde{m}_{1,1} - m_{0,0}\tilde{m}_{4,4}\tilde{m}_{3,3} + \tilde{m}_{2,2}m_{0,0}\tilde{m}_{5,5} + \tilde{m}_{3,3}^2\tilde{m}_{1,1} - \tilde{m}_{5,5}\tilde{m}_{1,1}^2 - \tilde{m}_{2,2}^2\tilde{m}_{3,3}}{\tilde{m}_{2,2}^3 - \tilde{m}_{2,2}\tilde{m}_{4,4}m_{0,0} - 2\tilde{m}_{2,2}\tilde{m}_{3,3}\tilde{m}_{1,1} + \tilde{m}_{3,3}^2m_{0,0} + \tilde{m}_{4,4}\tilde{m}_{1,1}^2} \tag{19}$$

$$\eta_1 = \frac{\tilde{m}_{2,2}\tilde{m}_{5,5}\tilde{m}_{1,1} + m_{0,0}\tilde{m}_{4,4}^2 - \tilde{m}_{0,0}\tilde{m}_{5,5}\tilde{m}_{3,3} - \tilde{m}_{4,4}\tilde{m}_{3,3}\tilde{m}_{1,1} - \tilde{m}_{2,2}^2\tilde{m}_{4,4} + \tilde{m}_{2,2}\tilde{m}_{3,3}^2}{\tilde{m}_{2,2}^3 - \tilde{m}_{2,2}\tilde{m}_{4,4}m_{0,0} - 2\tilde{m}_{2,2}\tilde{m}_{3,3}\tilde{m}_{1,1} + \tilde{m}_{3,3}^2m_{0,0} + \tilde{m}_{4,4}\tilde{m}_{1,1}^2} \tag{20}$$

$$\eta_0 = \frac{2\tilde{m}_{2,2}\tilde{m}_{4,4}\tilde{m}_{3,3} - \tilde{m}_{2,2}^2\tilde{m}_{5,5} - \tilde{m}_{3,3}^3 - \tilde{m}_{4,4}^2\tilde{m}_{1,1} + \tilde{m}_{5,5}\tilde{m}_{3,3}\tilde{m}_{1,1}}{\tilde{m}_{2,2}^3 - \tilde{m}_{2,2}\tilde{m}_{4,4}m_{0,0} - 2\tilde{m}_{2,2}\tilde{m}_{3,3}\tilde{m}_{1,1} + \tilde{m}_{3,3}^2m_{0,0} + \tilde{m}_{4,4}\tilde{m}_{1,1}^2} \tag{21}$$

Here, $\tilde{m}_{1,1}, \tilde{m}_{2,2}, \tilde{m}_{3,3}$ are given by Eqs. (12), (15) and (16). Moreover

$$\tilde{m}_{4,4} = m_{4,0} + m_{0,4} + 6(m_{2,2} + 2(m_{3,2} + m_{2,3} + m_{3,3}) + m_{4,2} + m_{2,4}) + 4(m_{1,3} + m_{3,1} + m_{4,1} + m_{1,4} + m_{4,3} + m_{3,4}) + m_{4,4} \tag{22}$$

$$\begin{aligned}\tilde{m}_{5,5} &= m_{5,0} + m_{0,5} + 5(m_{4,1} + m_{1,4} + m_{5,1} + m_{1,5} + m_{5,4} + m_{4,5}) + m_{5,5} + 10(m_{3,2} + m_{2,3} \\ &+ 3(m_{3,3} + m_{4,3} + m_{3,4}) + 2(m_{4,2} + m_{2,4} + m_{4,4}) + m_{5,2} + m_{2,5} + m_{5,3} + m_{3,5})\end{aligned} \tag{23}$$

The roots of the polynomial in Eq. (18) are z_j and the corresponding weights w_j can be calculated by using the expression (Press *et al*. [20])

$$w_j = \frac{<p_{N-1}/p_{N-1}>}{p_{N-1}(z_j)p'_N(z_j)},\ j = 1,2,........,N \tag{24}$$

Thus, $z_j = x_j + x_jy_j + y_j$ and w_j are known. The next step is to find the abscissas x_j and y_j. For that purpose three more equations are needed as given below:

$$\tilde{m}_{2,1} = \sum_{j=1}^{3} x_i^2 y_i w_i = x_1z_1w_1 + x_2z_2w_2 + x_3z_3w_3 \tag{25}$$

$$\tilde{m}_{3,2} = \sum_{j=1}^{3} x_i^3 y_i^2 w_i = x_1z_1^2w_1 + x_2z_2^2w_2 + x_3z_3^2w_3 \tag{26}$$

$$\tilde{m}_{4,3} = \sum_{j=1}^{3} x_i^4 y_i^3 w_i = x_1z_1^3w_1 + x_2z_2^3w_2 + x_3z_3^3w_3 \tag{27}$$

where

$$\tilde{m}_{2,1} = m_{2,0} + m_{2,1} + m_{1,1} \tag{28}$$

$$\tilde{m}_{3,2} = m_{3,0} + m_{1,2} + 2(m_{3,1} + m_{2,2} + m_{2,1}) + m_{3,2} \tag{29}$$

$$\begin{aligned}\tilde{m}_{4,3} &= m_{4,0} + m_{1,3} + 3(m_{2,2} + m_{2,3} + m_{3,1} \\ &+ 2m_{3,2} + m_{3,3} + m_{4,1} + m_{4,2}) + m_{4,3}\end{aligned} \tag{30}$$

The solution of the Eqs. (25)-(27) for x_j gives

$$x_1 = \frac{\tilde{m}_{4,3} - (z_2 + z_3)\tilde{m}_{3,2} + z_2 z_3 \tilde{m}_{2,1}}{z_1 w_1 (z_1 - z_2)(z_1 - z_3)}$$

$$x_2 = \frac{\tilde{m}_{4,3} - (z_1 + z_3)\tilde{m}_{3,2} + z_1 z_3 \tilde{m}_{2,1}}{z_2 w_2 (z_2 - z_3)(z_2 - z_1)}$$

$$x_3 = \frac{\tilde{m}_{4,3} - (z_1 + z_3)\tilde{m}_{3,2} + z_1 z_2 \tilde{m}_{2,1}}{z_3 w_3 (z_3 - z_1)(z_3 - z_2)}$$

Then

$$y_1 = \frac{z_1 - x_1}{1 + x_1}, y_2 = \frac{z_2 - x_2}{1 + x_2}, y_3 = \frac{z_3 - x_3}{1 + x_3} \qquad (31)$$

Finally, the resulting system of ordinary differential equations (ODEs) in (3) can be solved by a standard ODE-solver, for example a Runge-Kutta method.

NUMERICAL TEST PROBLEMS

In this section, two numerical test problems are presented. The numerical results of our scheme are compared with available analytical results. In both the test problems, symbols are used for the QMOM results and lines are used for the analytical solutions.

Problem 1: Bivariate aggregation with exponential initial distribution and constant kernel.

In this problem the two-component aggregation with exponential initial distribution and constant kernel is discussed. A square mesh of 50×50 mesh points and a geometric grid of the form

$$x_i = 2^{(i-N_x)/3} x_{max}, y_j = 2^{(j-N_y)/3} y_{max}, i, j = 0,1,2,..... \qquad (32)$$

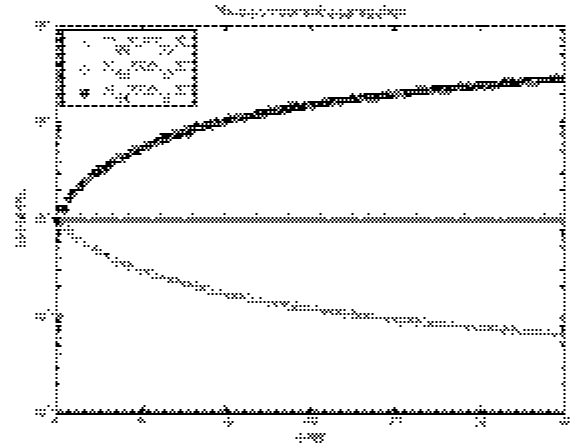
were considered. Here, N_x, N_y represent the number of mesh points in the x- and y-directions and x_{max}, y_{max} denote the maximum volumes (size) in each direction. The initial data is taken as

$$n(0,x,y) = \frac{N_0}{x_0 y_0} \exp\left(-\frac{x}{x_0} - \frac{y}{y_0}\right) \qquad (33)$$

and the analytical solution is given as (Lushnikov [22])

$$n(t,x,y) = \frac{4N_0}{(\tau+2)^2 x_0 y_0} \exp\left(-\frac{x}{x_0} - \frac{y}{y_0}\right) I_0(\theta) \qquad (34)$$

with $\theta = \left(\frac{4N_0 x y \tau}{(\tau+2) x_0 y_0}\right)^{\frac{1}{2}}$



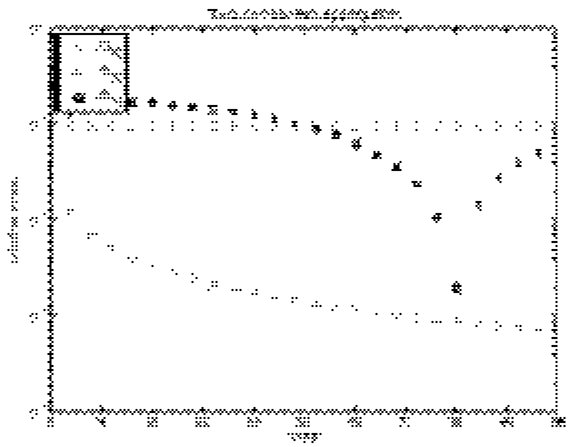


Fig. 1: (Case 1): Bivariate aggregation with constant kernel

Here, $\tau = \beta_0 N_0 t$ and I_0 is the modified Bessel function of first kind of order zero. The numerical results of QMOM are plotted against the analytical solutions. Figure 1 shows that the numerical results of our scheme are in good agreement with the analytical ones. However, one can see an over estimation in the result of $\tau = 100$.

Problem 2: Bivariate aggregation with Gaussian-type initial distribution and constant kernel.

Here, we used the same mesh points and geometric grid as discussed in previous problem. The initial distribution is given as

$$n(0,x,y) = \frac{16N_0}{x_0 y_0}\left(\frac{x}{x_0}\right)\left(\frac{y}{y_0}\right) \exp\left(-\frac{2x}{x_0} - \frac{2y}{y_0}\right) \qquad (35)$$

and the analytical solution is given as Gelbard *et al*. [23]

$$n(t,x,y) = \frac{8N_0}{x_0 y_0 \sqrt{\tau(\tau+2)^3}} \exp\left(-\frac{2x}{x_0} - \frac{2y}{y_0}\right) [I_0(\theta) - J_0(\theta)] \qquad (36)$$

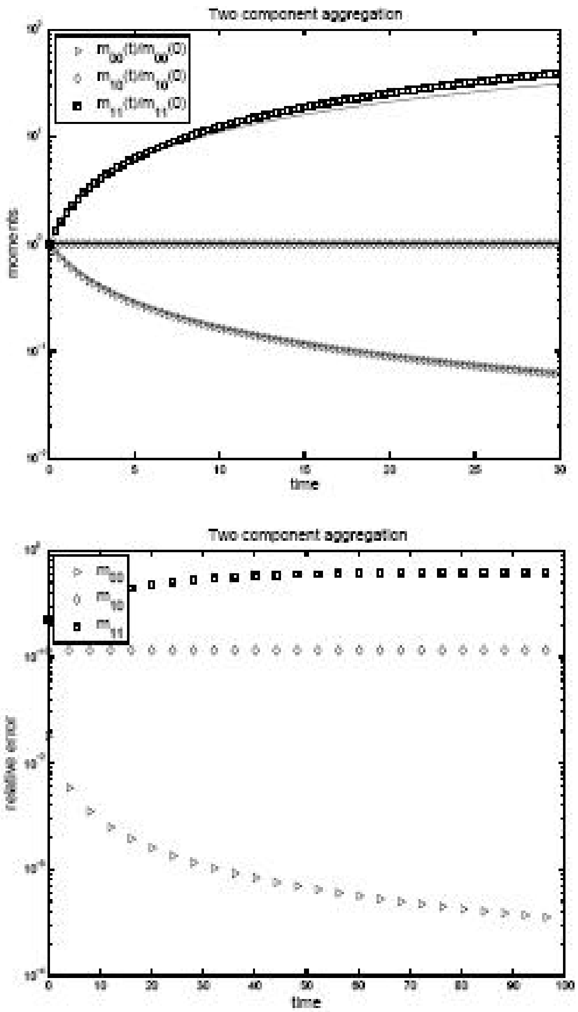


Fig. 2: (Case 2): Bivariate aggregation and Gaussian-type initial distribution

with

$$\theta = 4\left(\frac{xy}{x_0y_0}\right)^{\frac{1}{2}}\left(\frac{\tau}{\tau+2}\right)^{\frac{1}{4}}$$

Here, $\tau = \beta_0 N_0 t$ and I_0 and J_0 be the Bessel function and the modified Bessel functions of first kind of order zero respectively. For the numerical calculations we take $N_0 = 1$, $x_0 = 1$ and $y_0 = 1$. The numerical results are again comparable with the analytical results and results are shown in Fig. 2. A good agreement was found in the results.

CONCLUSIONS

In this article a different approach of QMOM was introduced for solving volume-based bivariate population balance equation. The technique is based on orthogonal polynomials of lower order moments which are used to calculate abscissas and weights. In this work, a third order polynomial is chosen, that requires first 36-moments for bivariate PBE to calculate pairs of quadrature points and weights. The required number of moments varies with the order of polynomial. Numerical test problems for two-component PBE with different initial distributions were carried out for demonstrating the accuracy of current technique. Numerical approximations obtained by our proposed technique were plotted against the exact solutions. Fairly good agreements were observed in all test problems. The error analysis showed that QMOM has approximated the given models accurately. The integral of nucleation term is free of the number density function, therefore QMOM is not applicable. For that reason an accurate approximation of the nucleation integral is desirable for overall accuracy of the method.

ACKNOWLEDGNENT

The first author is thankful to University of Engineering & Technology Peshawar (Mardan Campus) for providing research facilities.

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