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A Numerical Approach to Solve Volume-Based Batch Crystallization Model with Fines Dissolution Unit

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Abstract: In this article, a numerical study of a one-dimensional, volume-based batch crystallization model (PBM) is presented that is used in numerous industries and chemical engineering sciences. A numerical approximation of the underlying model is discussed by using an alternative Quadrature Method of Moments (QMOM). Fines dissolution term is also incorporated in the governing equation for improvement of product quality and removal of undesirable particles. The moment-generating function is introduced in order to apply the QMOM. To find the quadrature abscissas, an orthogonal polynomial of degree three is derived. To verify the efficiency and accuracy of the proposed technique, two test problems are discussed. The numerical results obtained by the proposed scheme are plotted versus the analytical solutions. Thus, these findings line up well with the analytical findings.

Keywords: volume-based population balance model with fines dissolution; quadrature method of moments; orthogonal polynomials

1. Introduction

Population balance models (PBMs) show a significant role in different areas of science and engineering. These models have numerous applications in high-energy physics, geophysics, biophysics, meteorology, pharmacy, food science, chromatography, chemical engineering, civil engineering, and environmental engineering. These models are used in the process of cell dynamics, polymerization, cloud formation, and crystallization. In biophysics, these models are concerned with population of various kinds of cells. Population balance models are also used in the formation of ceramics mixtures and nanoparticles which have a lot of applications.

In 1964, Hulburt & Katz [1] were first to discuss the PBMs in chemical engineering. A detailed description of these models is given in [2]. The main components in the models are the process of nucleation, growth, aggregation, breakage, inlet, outlet, growth, and dissolution. The mathematical model of population balance equations are partial integro-differential equations (PIDEs). Analytical solutions of these PIDEs are very rare except for a few simple cases. Therefore, researchers are interested in developing numerical solutions for these equations. Numerous numerical methods are accessible in the literature to solve certain kinds of PBMs; see, for example, [3–11].

The Quadrature Method of Moments (QMOM) for solving the governed models was first introduced by McGraw [12]. The direct QMOM was proposed by Fan et al. [4]. In addition, a new QMOM has been proposed by Gimbun [5]. Qamar et al. [13] introduced an alternative QMOM for solving length-based batch crystallization models telling crystals nucleation, size-dependent growth, aggregation, breakage, and dissolution of small nuclei below certain critical size. Safyan et al. [14] followed the technique of [13] for solving volume-based batch crystallization model nucleation,

size-dependent growth, aggregation, breakage. In this article, the QMOM is used to solve volume-based batch crystallization models with fines dissolution. The fines dissolution unit improves the product quality and removes unwanted particles.

In the proposed method, orthogonal polynomials, taken from the lower-order moments, are used to find the quadrature points and weights. For confirming accuracy of the scheme, a third-order orthogonal polynomial, employing the first six moments, was chosen to estimate the quadrature points (abscissas) and equivalent quadrature weights. Hence, it was essential to solve at least a six-moment system (i.e., 0, ... , 5). This type of polynomial provides a three-point Gaussian quadrature rule which usually produces precise output for polynomials of degree five or less. The expression for the preferred orthogonal polynomial can be derived analytically and the mandatory number of moments rises with order of polynomial. It is important to mention that the calculation of six moments to generate each time the third-order polynomial is compulsory. However, the technique itself is not limited to the calculation of every listed number of moments. The calculation of additional moments is conducted by adding ordinary differential equation.

This article is divided into two parts: In the first part, the mathematical model of volume-based Population Balance Equation (PBE) with fines dissolution is presented. In the second part, the proposed QMOM is derived for PBEs. Furthermore, the mathematical outcomes of QMOM are compared with the analytical outcomes that are accessible in literature.

2. Materials and Methods

Suppose u_d represents the number density function, then a general PBE is given by [1,2]:

$$\frac{\partial u_d(T,V_p)}{\partial T} = \underbrace{-\frac{\partial[G(T,V_p)u_d(T,V_p)]}{\partial V_p}}_{\text{Growth-term}} + \underbrace{Q_{nuc}(T,V_p)}_{\text{Nucleation-term}} + \underbrace{Q^{\pm}_{\text{agg}}(T,V_p)}_{\text{Aggregation-term}} + \underbrace{Q^{\pm}_{\text{break}}(T,V_p)}_{\text{Breakage-term}} + \underbrace{Q_{\text{diss}}(T,V_p)}_{\text{Dissolution-term}} \quad (1)$$
$$u_d\big(0,V_p\big) = u_{d0}\big(V_p\big) \quad \big(T,V_p\big) \in R^2_+$$

where $\mathbb{R}_+ = (0,\infty)$. The variable T represents the time and V_p may be size, length, or composition. In this article, it represents the particle volume. In the above equation, each term has its specific definition. These terms are given by

$$Q^{\pm}_{\text{agg}}(T,V_p) = B_{\text{agg}}(T,V_p) - D_{\text{agg}}(T,V_p) \quad (2)$$

where

$$B_{\text{agg}}\big(T,V_p\big) = \frac{1}{2}\int_0^{V_p} \beta\big(T,V_p - V'_p, V'_p\big)u_d\big(T,V_p - V'_p\big)u_d\big(T,V'_p\big)dV'_p$$

and

$$D_{\text{agg}}\big(T,V_p\big) = \int_0^{\infty} \beta\big(T,V_p,V'_p\big)u_d\big(T,V_p\big)u_d\big(T,V'_p\big)dV'_p$$

Here, $B_{\text{agg}}\big(T,V_p\big)$ represents the birth of particles of volume V_p resulting for amalgamation of two particles with respective volume V'_p and $V_p - V'_p$, where $V'_p \in \big(0,\ V_p\big)$ and $D_{\text{agg}}\big(T,V_p\big)$ is the death of particles, describing the decrease in particle volume V_p by aggregation with other particles of any volume. The aggregation kernel $\beta\big(T,V_p,V'_p\big)$ is the rate at which aggregation of two particles V_p and V'_p produces a particle volume $V_p + V'_p$.

$$Q^{\pm}_{\text{break}}(T,V_p) = B_{\text{break}}(T,V_p) - D_{\text{break}}(T,V_p) \quad (3)$$

where

$$B_{\text{break}}\left(T, V_p\right) = \int_{V_p}^{\infty} b\left(T, V_p, V_p'\right) S\left(V_p'\right) u_d\left(T, V_p'\right) dV_p'$$

and

$$D_{\text{break}}(T, V_p) = S(V_p) u_d(T, V_p)$$

Here, $B_{\text{break}}\left(T, V_p\right)$ represents the birth of new particles during the breakage process and the breakage function $b\left(T, V_p, V_p'\right)$ is the probability density function for the formation of particle volume V_p from particle volume V_p', whereas, $D_{\text{break}}\left(T, V_p\right)$ is the death of particles, and $S\left(V_p'\right)$ is the selection function describing the rate at which the particles are selected to break.

$$Q_{\text{diss}}\left(T, V_p\right) = \frac{\dot{V}}{V_c} h\left(V_p\right) u_d\left(T, V_p\right) \tag{4}$$

$Q_{\text{diss}}\left(T, V_p\right)$ represents the dissolution term, V_c is the volume of crystallizer, $\dot{V}$ is the volumetric flow rate from the crystallizer to dissolution unit, $h\left(V_p\right)$ is the dissolution function describing dissolution of small particles below some critical size. The population balance equation can be simplified through introducing the moment function. The kth moment of the population density function is mathematically written in the form:

$$m_k(T) = \int_0^{\infty} V_p^k u_d(T, V_p) dV_p \tag{5}$$

The first and second moments $m_0(T)$, $m_1(T)$ denote particle population and volume, respectively, at any instant T. Multiply V_p^k to left- and right-hand side of Equation (1) and at that moment integrate it over the volume V_p, so we obtain the following equation:

$$\frac{dm_k(T)}{dT} = \overline{G_{\text{growth}}}(T, V_p) + \overline{Q_{\text{nucleation}}}(T, V_p) + \overline{Q_{\text{aggregation}}}(T, V_p) + \overline{Q_{\text{breakage}}}(T, V_p) + \overline{Q_{\text{dissolution}}}(T, V_p) \tag{6}$$

where

$$\overline{G_{\text{growth}}}(T, V_p) = \int_0^{\infty} V_p^k \frac{\partial [G(T, V_p) u_d(T, V_p)]}{\partial V_p} dV_p$$

$$\overline{Q_{\text{nucleation}}}(T, V_p) = \int_0^{\infty} V_p^k Q_{nuc}(T, V_p) dV_p$$

$$\overline{Q_{\text{aggregation}}}(T, V_p) = \overline{B_{\text{agg}}}(T, V_p) - \overline{D_{\text{agg}}}(T, V_p)$$

The aggregation terms $\overline{B_{\text{agg}}}(T, V_p)$ and $\overline{D_{\text{agg}}}(T, V_p)$ are mathematically defined as

$$\overline{B_{\text{agg}}}\left(T, V_p\right) = \frac{1}{2} \int_0^{\infty} V_p^k \int_0^{V_p} \beta\left(T, V_p - V_p', V_p'\right) u_d\left(T, V_p - V_p'\right) u_d\left(T, V_p'\right) dV_p' dV_p$$

$$\overline{D_{\text{agg}}}\left(T, V_p\right) = \int_0^{\infty} V_p^k u_d\left(T, V_p\right) \int_0^{\infty} \beta\left(T, V_p, V_p'\right) u_d\left(T, V_p'\right) dV_p' dV_p$$

$$\overline{Q_{\text{breakage}}}(T, V_p) = \overline{B_{\text{break}}}(T, V_p) - \overline{D_{\text{break}}}(T, V_p)$$

whereas $\overline{B_{\text{break}}}(T, V_p)$ and $\overline{D_{\text{break}}}(T, V_p)$ are birth and death functions because of breakage term and are given by

$$\overline{B_{\text{break}}}\left(T, V_p\right) = \int_0^\infty V_p^k \int_{V_p}^\infty b\left(T, V_p, V_p'\right) S\left(V_p'\right) u_d\left(T, V_p'\right) dV_p' dV_p$$

$$\overline{B_{\text{break}}}\left(T, V_p\right) = \int_0^\infty V_p^k S\left(V_p\right) u_d\left(T, V_p\right) dV_p$$

$$\overline{Q_{\text{dissolution}}}\left(T, V_p\right) = \frac{\dot{V}}{V_c} \int_0^\infty V_p^k h\left(V_p\right) u_d\left(T, V_p\right) dV_p$$

Due to aggregation, the upper limit in the birth function is not infinity; therefore, we cannot apply quadrature method of moment for this integral. To apply the QMOM, we have to convert the upper limit to infinity. Here, we introduce a Heaviside step function $H\left(V_p - V_p'\right)$ to solve the integral such that $H\left(V_p - V_p'\right) = 0$ when $V_p - V_p' < 0$ and $H\left(V_p - V_p'\right) = 1$ otherwise. As a result, we will find the limits of integration over V_p' from $\left(0, V_p\right)$ to $(0, \infty)$. Thus, by applying it to the birth function, we obtain the following equation:

$$\begin{aligned} &\tfrac{1}{2} \int_0^\infty V_p^k dV_p \int_0^\infty H\left(V_p - V_p'\right) \beta\left(T, V_p - V_p', V_p'\right) u_d\left(T, V_p - V_p'\right) u_d\left(T, V_p'\right) dV_p' \\ &\quad = \tfrac{1}{2} \int_0^\infty u_d\left(T, V_p'\right) dV_p' \int_0^\infty \left(u + V_p'\right)^k \beta\left(T, u, V_p'\right) u_d(T, u) dV_p \end{aligned} \tag{7}$$

On the right side of Equation (7), we have switched the order of integration and made the replacement $u = V_p - V_p'$. Lastly, we have replaced V_p for u with no damage of generality and caught the necessary outcome for birth due to aggregation which is given by

$$\overline{B_{\text{agg}}}(T, V_p) = \frac{1}{2} \int_0^\infty u_d(T, V'_p) \int_0^\infty (V_p + V'_p)^k \beta(T, V_p, V'_p) u_d(T, V_p) dV_p dV'_p$$

After substituting all of the above terms in Equation (6), we get the system of differential equations:

$$\begin{aligned} \tfrac{dm_k(T)}{dT} &= \int_0^\infty k V_p^{k-1} G\left(T, V_p\right) u_d\left(T, V_p\right) dV_p + \int_0^\infty V_p^k Q_{nuc}\left(T, V_p\right) dV_p \\ &+ \tfrac{1}{2} \int_0^\infty u_d\left(T, V_p'\right) \int_0^\infty \left(V_p + V_p'\right)^k \beta\left(T, V_p, V_p'\right) u_d\left(T, V_p\right) dV_p dV_p' \\ &- \int_0^\infty V_p^k u_d\left(T, V_p\right) \int_0^\infty \beta\left(T, V_p, V_p'\right) u_d\left(T, V_p'\right) dV_p' dV_p \\ &+ \int_0^\infty V_p^k \int_{V_p}^\infty b\left(T, V_p, V_p'\right) S\left(V_p'\right) u_d\left(T, V_p'\right) dV_p' dV_p \\ &- \int_0^\infty V_p^k S\left(V_p\right) u_d\left(T, V_p\right) dV_p + \tfrac{\dot{V}}{V_c} \int_0^\infty V_p^k h\left(V_p\right) u_d\left(T, V_p\right) dV_p \end{aligned} \tag{8}$$

In addition, with solid phase, the liquid phase yields ordinary differential equation for the solute mass in the form:

$$\frac{dm(T)}{dT} = \dot{m}_{\text{in}}(T) - \dot{m}_{\text{out}}(T) - 3\sigma_c k_v \int_0^\infty V_p^2 G\left(T,\ V_p\right) u_d\left(T, V_p\right) dV_p \tag{9}$$

with $m(0) = m_0$ where σ_c is the density of crystals and k_v is a volume shape factor. $\dot{m}_{\text{in}}(T) - \dot{m}_{\text{in}}(T)-$ is the incoming mass flux from dissolution unit to crystallizer and outgoing mass flux from crystallizer to dissolution unit, respectively, which is mathematically defined by

$$\dot{m}_{\text{out}}(T) = \frac{m(T)}{m(T) + m_{\text{solv}}(T)} \sigma_{sol}(T)\dot{V} \tag{10}$$

where $m_{\text{solv}}(T)$ is the mass of solvent and $\sigma_{sol}(T)$ is the density of the solution. $T_p = \frac{V_p}{V} \geq 0$ is the residence time in the dissolution unit, where V_p represents volume of the pipe.

Here, we will consider the Gaussian quadrature method to solve the complicated integral terms appearing in Equations (8) and (9). Consequently, a closed-form system of moments is found. Further, we have accurately and efficiently solved the closed-form system with an ODE solver. The approximation of definite integral with the help of quadrature rule is an important numerical aspect. For this purpose, first we calculate the function at definite points and then use the formula of weight function which gives approximation of the definite integral. To approximate a definite integral given in Equations (8) and (9), first we find the values of the function at a set of equidistant points. After evaluating, the weight function is multiplied to approximate the integrals. In this rule, there is no limitation of choosing abscissas and weights. This rule also works for the points which are not likewise spread out. Let us assume the integral of the formula $\int_a^b \psi\left(V_p\right) u_d\left(V_p\right) dV_p$. We can find the weights w_j and abscissas V_{kp_i} by approximating the definite integral as

$$\int_a^b \psi(V_p) u_d(V_p) dV_p = \sum_{j=1}^{N} w_j u_d(V_{p_j}) \tag{11}$$

where provided it is exact and $u_d\left(V_p\right)$ is smooth function. A set of orthogonal polynomials is necessary for making certain n^{th} order orthogonal polynomial and it should contain only one polynomial of order j for $j = 1, 2, 3, \ldots$. We can define the scalar product of the two functions $k\left(V_p\right)$ and $h\left(V_p\right)$ over a weight function $\psi\left(V_p\right)$ by

$$< h \backslash k >= \int_a^b \psi(V_p) h(V_p) k(V_p) dV_p \tag{12}$$

If we find the zero scalar product of any two functions h and k, then these functions are termed as orthogonal functions. It is also noted that supplementary information will be required for obtaining abscissas and weights if the classical weight function $\psi\left(V_p\right)$ is not provided. For this purpose, we have used the moment:

$$m_i(T) = \int_0^\infty V_p^i u_d(T, V_p) dV_p \approx \sum_{j=1}^{N} V_{p_j}^j w_j \tag{13}$$

In the above equation, $u_d\left(T,\ V_p\right)$ is used as a weight function $\psi\left(V_p\right)$. V_p^i given in Equation (13) denotes the polynomial $u_d\left(\ V_p\right)$ of ith order. To find n abscissas weights, we need $2n$ moments from m_0 to m_{2n-1}. For $i \leq 2n-1$ this approximation will be exact. For simplicity and accurate approximations, we set $n = 3$. As a result, six-moment system for $m_0, \ldots\ldots, m_5$ is calculated. To discuss the procedure, we consider ODEs (8) and (9). Using Equation (13) in Equations (8) and (9), we obtain the following equations:

$$\begin{aligned}\frac{dm_k(T)}{dT} &= k\sum_{i=1}^{N}\left(V_{p_i}\right)^{k-1}w_iG\left(T,\ V_{p_i}\right)+a_{nuc}^{(k)}\\ &+\tfrac{1}{2}\sum_{i=1}^{N}w_i\sum_{j=1}^{N}\left(V_{p_i}+V_{p_j}\right)^k\beta\left(T,V_{p_i},V_{p_j}\right)w_j\\ &-\sum_{i=1}^{N}\left(V_{p_i}\right)^k w_i\sum_{j=1}^{N}\beta\left(T,V_{p_i},V_{p_j}\right)w_j\\ &+\sum_{i=1}^{N}\left(V_{p_i}\right)^k w_i\sum_{j=1}^{N}\beta\left(T,V_{p_i},V_{p_j}\right)S\left(V_{p_j}\right)w_j\\ &+\tfrac{\dot{V}}{V_c}\sum_{i=1}^{N}w_i\left(V_{p_i}\right)^k h\left(V_{p_i}\right)\qquad k=0,1,2,\ldots\ldots\end{aligned}\tag{14}$$

where $a_{nuc}^{(k)}=\int_0^\infty {V_p}^k Q_{nuc}dV_p$ and

$$\frac{dm(T)}{dT}=\dot{m}_{\text{in}}(T)-\dot{m}_{\text{out}}(T)-3\sigma_c k_v\sum_{i}^{N}w_iV_p^2G\left(T,\ V_{p_i}\right)\tag{15}$$

Our next step is computing the quadrature points $V_{pi},\ V'_{pj}$ and the quadrature weights w_i and w_j. The quadrature points $V_{pi},\ V'_{pj}$ are obtained from the roots of orthogonal polynomials. The construction of orthogonal polynomials is described as follows:

$$p_{-1}=0, p_0=1, p_j=(V_p-\alpha_j)p_{j-1}-\beta_jp_{j-1}\tag{16}$$

with

$$\alpha_j=\frac{<V_pp_{j-1}/p_{j-1}>}{<p_{j-1}/p_{j-1}>}, j=1,2,\ldots.\tag{17}$$

$$\beta_j=\frac{<p_{j-1}/p_{j-1}>}{<p_{j-2}/p_{j-2}>}, j=2,3,\ldots.\tag{18}$$

Since the function $u_d\left(T,\ V_p\right)$ is used as a weight function $\psi\left(V_p\right)$, so from Equation (12) we have

$$<p_j/p_j>=\int_a^b u_d(T,V_p)p_j^2dV_p$$

Using all of the above definitions, the orthogonal polynomials of any order can be obtained. Our first step is to find the roots of the nth order polynomial. The quadrature points V_p are then obtained from these roots. To explain the procedure of deriving these orthogonal polynomials, we have calculated $p_1\left(V_p\right), p_2\left(V_p\right),\ p_3\left(V_p\right)$. $p_1\left(V_p\right)$ as

$$p_1(V_p)=(V_p-\alpha_1)p_0=(V_p-\alpha_1)$$

First, α_1 will be calculated, which is given by

$$\alpha_1=\frac{<V_pp_0/p_0>}{<p_0/p_0>}=\frac{\int_0^\infty V_pu_d(T,V_p)p_0^2dV_p}{\int_0^\infty u_d(T,V_p)p_0^2dV_p}=\frac{m_1(T)}{m_0(T)}$$

so

$$p_1(V_p)=V_p-\frac{m_1}{m_0}\tag{19}$$

Now

$$p_2(V_p) = (V_p - \alpha_2)p_1 - \beta_2 p_1 \tag{20}$$

Again from Equations (17) and (18) we have

$$\alpha_2 = \frac{<V_p p_1/p_1>}{<p_1/p_1>} = \frac{\int_0^\infty V_p u_d(T,V_p) p_1^2 dV_p}{\int_0^\infty u_d(T,V_p) p_1^2 dV_p} = \frac{\int_0^\infty V_p u_d(T,V_p)\left(V_p - \frac{m_1}{m_0}\right)^2 dV_p}{\int_0^\infty u_d(T,V_p)\left(V_p - \frac{m_1}{m_0}\right)^2 dV_p} = \frac{m_3 m_0^2 - 2m_0 m_1 m_2 + m_1^3}{m_2 m_0^2 - m_0 m_1^2} \tag{21}$$

and

$$\beta_2 = \frac{< p_1/p_1 >}{< p_0/p_0 >} = \frac{\int_0^\infty V_p u_d(T,V_p)\left(V_p - \frac{m_1}{m_0}\right)^2 dV_p}{\int_0^\infty u_d(T,V_p) dV_p} = \frac{m_2 m_0 - m_1^2}{m_0^2} \tag{22}$$

so from Equation (20) we have

$$p_2(V_p) = \frac{{V_p}^2(m_0 m_2 - m_1^2) + V_p(m_1 m_2 - m_0 m_3) + m_1 m_3 - m_2^2}{m_0 m_2 - m_1^2} \tag{23}$$

Proceeding in a similar way, we can calculate the polynomial of higher order. The third-order polynomial $p_3\left(V_p\right)$ is given by the following equation:

$$\begin{aligned} p_3(V_p) &= {V_p}^3 + \frac{(m_2 m_4 m_1 - m_0 m_4 m_3 + m_2 m_0 m_5 + m_3^2 m_1 - m_5 m_1^2 - m_2^2 m_3){V_p}^2}{m_2^3 - m_2 m_4 m_0 - 2m_2 m_3 m_1 + m_3^2 m_0 + m_4 m_1^2} \\ &+ \frac{(m_2 m_5 m_1 + m_0 m_4^2 - m_0 m_5 m_3 - m_4 m_3 m_1 - m_2^2 m_4 + m_3^2 m_2)V_p}{m_2^3 - m_2 m_4 m_0 - 2m_2 m_3 m_1 + m_3^2 m_0 + m_4 m_1^2} + \frac{2m_2 m_4 m_3 - m_2^2 m_5 - m_3^3 - m_4^2 m_1 + m_5 m_3 m_1)}{m_2^3 - m_2 m_4 m_0 - 2m_2 m_3 m_1 + m_3^2 m_0 + m_4 m_1^2} \end{aligned} \tag{24}$$

The roots of the selected polynomial will give us the abscissas V_p. Next, the weights w_i will be calculated. According to Press et al. [15], the expression for the weight function is given by

$$w_i = \frac{\langle p_{N-1}/p_{N-1}\rangle}{p_{N-1}\left(x_j\right)p'_N\left(x_j\right)} \qquad i = 1, 2, \ldots\ldots\ldots N \tag{25}$$

where N is the order of the selected polynomial. At last, the resulting system of ODEs is then solved by any standard ODE solver in MatLab.

3. Results

Test Problem 1: Aggregation with Fines Dissolution

Here, the proposed scheme is analyzed for aggregation with fines dissolution (see Figure 1) problem encountered in several particulate methods (i.e., fluidized beds, formation of rain droplets, and manufacture of dry powders). The effects of further procedures, such as breakage, growth, and nucleation, are negligible. During the aggregation process, the total mass of particles m_1 is conserved and the amount of particles m_0 reduces during the processing time. The aggregation kernel is held to be constant and is defined as $\beta(V_p, V'_p) = \beta_0$, where $\beta_0 = 1$. The exponential initial particle size distribution is given by

$$u_d\left(0, V_p\right) = \frac{N_0}{V_{P_0}} exp\left(-V_p/V_{P_0}\right) \tag{26}$$

where $N_0 = 1$ and $V_{p0} = 1$. The dissolution term $h(V_p)$ explains the dissolution of particles below certain critical size, that is, $2 \times 10^{-4} m^3$. The analytical solution in terms of the number density $u_d(T, V_p)$ is given by Scott [16]:

$$u_d(T, V_p) = \frac{4N_0}{V_{P_0}(\tau + 2)^2} exp(-2V'_p/\tau + 2) \tag{27}$$

where $\tau = N_0 \beta_0 t$ and $V'_p = V/V_{p0}$. The plot in Figure 2 shows normalized moments. The outcomes of our QMOM are in decent agreement with analytical outcomes. It is also observed from Figure 2 that during the aggregation process, the number of particles $m_0(T)$ decreases while the volume of the particles $m_1(T)$ remains constant.

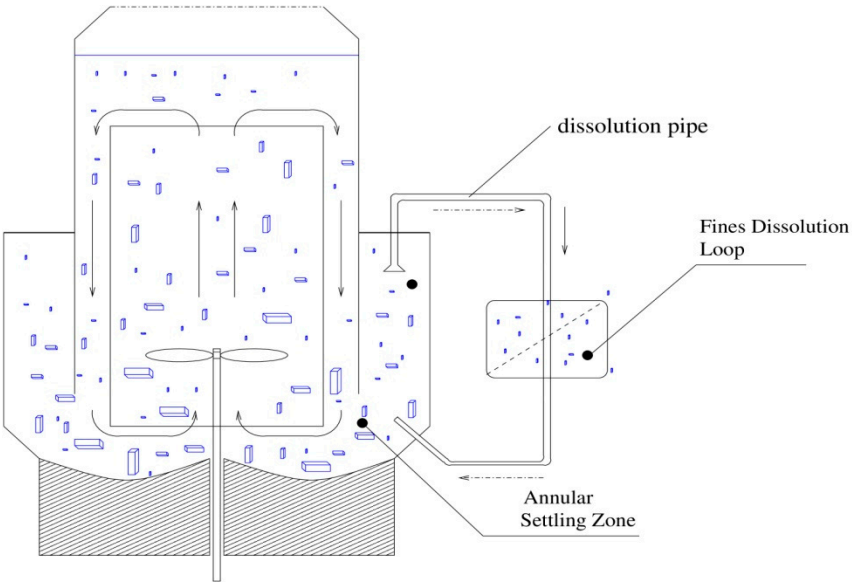

Figure 1. Single batch setup process with fines dissolution.

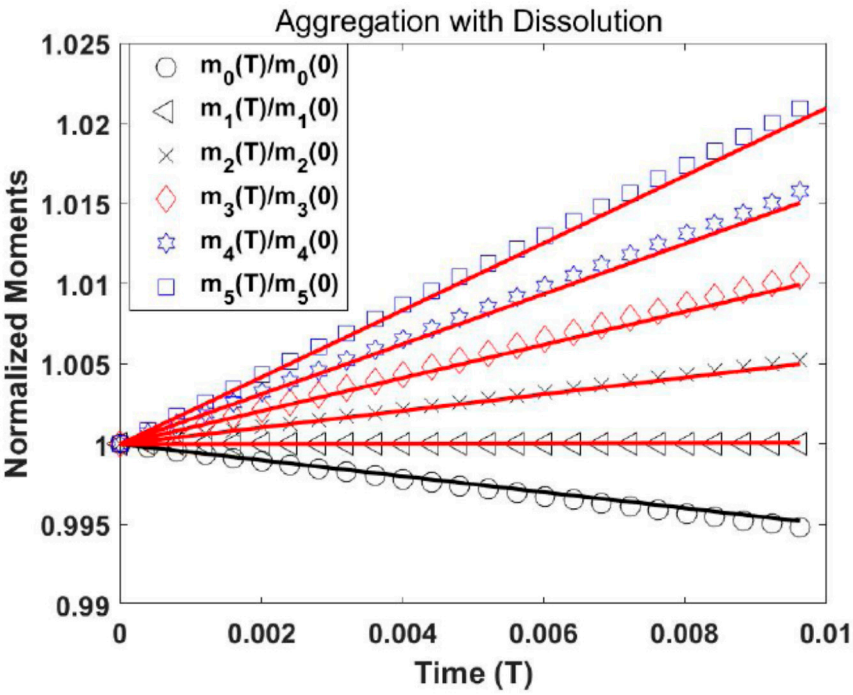

Figure 2. Aggregation with fines dissolution.

Test Problem 2: Aggregation and Breakage with Fines Dissolution

In this problem, we take a batch crystallizer in which aggregation and breakage are the main occurrences and which is connected with a fines dissolver. The growth and nucleation terms are neglected in this process. The initial distribution is given by

$$u_d\left(0, V_p\right) = M_0 \cdot \frac{M_0}{M_1} exp\left(-\frac{M_0}{M_1} V_p\right) \tag{28}$$

where, $M_0 = \frac{2N_0}{2+\beta_0 N_0 t}$ and $M_1 = N_0 V_{p0}\left[1 - \frac{2G_0}{\beta_0 N_0 V_{p0}} \ln\left(\frac{2}{2+\beta_0 N_0 t}\right)\right]$ represent the zero and first moments, respectively. A constant aggregation term, $\beta(V_p, V'_p) = \beta_0 = 1$, a breakage kernel $b(V_p, V'_p) = 2/V'_p$,, and uniform daughter distribution $S(V_p) = V_p$ are taken. The analytical solution is given by Patel [17]:

$$u_d\left(T, V_p\right) = \frac{M_0^2}{M_1} exp\left(-\frac{M_0}{M_1} V_p\right) \tag{29}$$

The numerical results are displayed in Figure 3. The moments of the numerical system are in good agreement with those taken from the analytical solution. It is also observed from Figure 3 that during the aggregation and breakage process, the number of particles $m_0(T)$ decreases while the volume of the particles $m_1(T)$ remains constant.

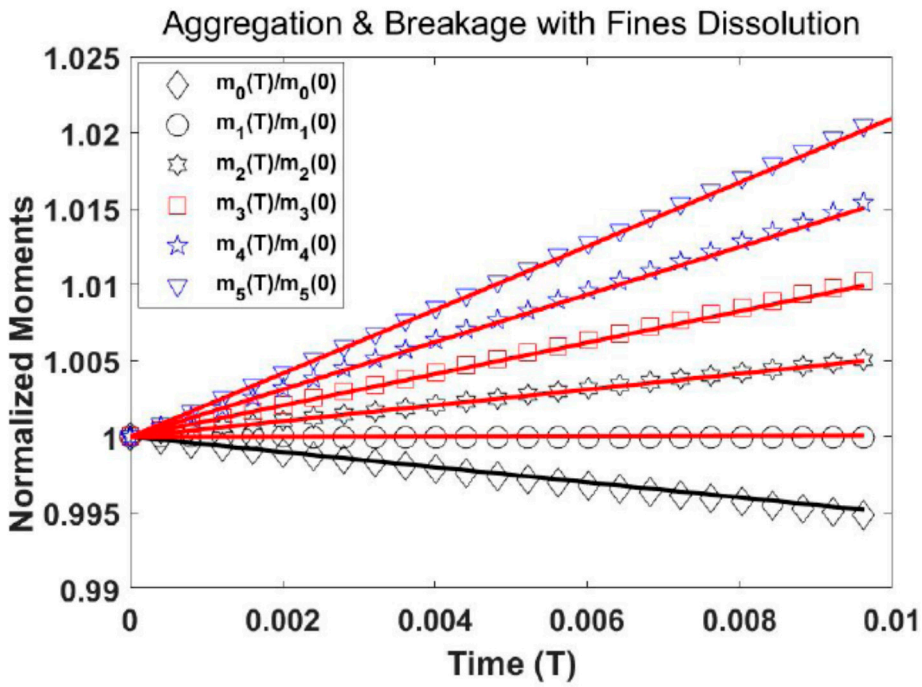

Figure 3. Aggregation and breakage with fines dissolution.

4. Conclusions

The moment-generating function was used to convert the governing partial differential equation into a system of ordinary differential equations. The mathematical term for fines dissolution was incorporated in the model for improving the quality of the product. The Gaussian quadrature method was implemented to solve the complicated integrals in this research. An orthogonal polynomial of degree three, which utilizes the first six moments, was used for better accuracy of the proposed scheme. To check the significance of the scheme, two case studies were discussed. The results of the proposed scheme are in perfect agreement with the available analytical results. No dissipation was observed in the results. This work is extendable for batch preferential crystallization models with fines dissolution.

Furthermore, the developed scheme could be applicable to solve multidimensional batch crystallization models with fines dissolution.

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