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# Analytical solution of population balance equation involving aggregation and breakage in terms of auxiliary equation method

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**Abstract.** This paper presents an effective analytical simulation to solve population balance equation (PBE), involving particulate aggregation and breakage, by making use of appropriate solution(s) of associated complementary equation via auxiliary equation method (AEM). Travelling wave solutions of the complementary equation of a nonlinear PBE with appropriately chosen parameters is taken to be analogous to the description of the dynamic behaviour of the particulate processes. For an initial proof-of-concept, a general case when the number of particles varies with respect to time is chosen. Three cases, i.e. (1) balanced aggregation and breakage, (2) when aggregation can dominate and (3) breakage can dominate, are selected and solved for their corresponding analytical solutions. The results are then compared with the available analytical solution, based on Laplace transform obtained from literature. In this communication, it is shown that the solution approach proposed via AEM is flexible and therefore more efficient than the analytical approach used in the literature.

Keywords. Population balance; aggregation; breakage; auxiliary equation method; Laplace transform.

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# 1. Introduction

A significant property of most of the particulate processes is the particle size, and the distribution of this property is a major characteristic of such processes which, as a result, affects the behaviour and performance of the final product. In general, particulate processes are characterized by size distributions that are assumed to vary strongly in time with

respect to the mean particle size and the shape of the particle size distribution (PSD). As a result, particulate phenomena like aggregation and breakage may occur during these processes which may result in momentous changes manifested through its PSD [1]. The time evolution of this PSD is determined by solving the so-called population balance equation (PBE) which governs the dynamic behaviour of particulate processes [2]. As a model, PBE essentially consists of a nonlinear partial integrodifferential equation encountered in numerous scientific and engineering disciplines with certain source and/or sink terms, typically referred to as kernels [2]. The numerical solution of such a dynamic population balance model (PBM), is a remarkably complex mathematical problem, due to both numerical complications and uncertainties of the model regarding the particulate mechanisms that are frequently weakly approximated. On the other hand, the essence of any numerical solution of a PBE requires the discretization of particle diameter/volume domain by means of certain numerical approximations that result in a system of stiff, nonlinear differential or algebraic/differential equations.

Since the early 1960s, various numerical methods have been developed to solve PBMs, involving both time-dependent and time-independent formulations. The fully discrete method [3–5], method of classes [6,7], fixed and moving pivot method [8,9], higher-order discretized method [10-13], orthogonal collocation on finite elements [14,15], Monte Carlo method [16], least squares method [17,18] are to name only a few. Despite numerous published papers on the numerical solution of the PBEs, the choice of the most appropriate method for calculating time evaluation of a PSD in processes undergoing aggregation and breakage is not straightforward and simple. In reality, a large number of published papers only refer to a limited range of variation of particle breakage and aggregation rates. Therefore, the wide-ranging application of a numerical method to solve a specific problem cannot be assured. What is more complicated is the fact that, exact analytical solutions cannot be obtained for most of the nonlinear differential problems that occur in nature. Broadly speaking, by an exact analytical solution it is meant that the solution is given in terms of functions whose properties are known or tabulated. Even when such a solution is present, it may not be particularly useful from either a computational or an analytical point of view. On the other hand, formulation of a large number of different numerical approaches also underlines the intrinsic problem in obtaining a precise and consistent solution method.

In this study, the analytical solution of a batch PBE as suggested by McCoy and Madras [19], in which the number of particles varies with respect to time, is compared with the analytical solution proposed by Pinar and Öziş [20,21]. The validity of the proposed method is established through case studies using relative weights of aggregation and breakage. The proposed analytical method involves the target solution of a nonlinear evolution equation to be expressed as a polynomial in an elementary function which satisfies a particular ordinary differential equation termed as auxiliary equation, in general, and is more flexible and thereby more efficient than the analytical approach used in the literature.

#### 2. Problem formulation

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Population balance equation (PBE) is a nonlinear partial integrodifferential equation encountered in numerous scientific and engineering disciplines [2]. The PBE describes

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the evolution of a density function, representing the behaviour of population of a state vector such as solid particles, liquid droplets or gas bubbles. The evolution of this density function takes into account different processes such as aggregation, breakage, growth and advective transport of the state vector that control the population. The batch PBE without considering spatial dependence and growth, based on the so-called LPA formulation as mentioned in McCoy and Madras [19] (analytical formulations of Lage [22], Patil and Andrews [23] are denoted here as LPA) can be written as

$$\frac{\partial n(v,t)}{\partial t} = \underbrace{\frac{1}{2} \int_{0}^{v} C(v',v-v')n(v',t)n(v-v',t)dv'}_{\text{BIRTH due to aggregation}} -\underbrace{\frac{n(v,t) \int_{0}^{\infty} C(v,v')n(v',t)dv'}_{\text{DEATH due to aggregation}}}_{\text{DEATH due to aggregation}} +\underbrace{2 \int_{v}^{\infty} \Omega(v,v')S(v')n(v',t)dv'}_{\text{DEATH due to breakage}} -\underbrace{S(v)n(v,t)}_{\text{DEATH due to breakage}}, \quad (1)$$

where n(v, t) is the number density function in terms of the particle volume v. C(v, v') is the volume-based aggregation kernel that describes the frequency at which particles with volume v and v' collide to form a particle of volume v + v', S(v) is the volume-based breakage function and the stoichiometric kernel  $\Omega(v, v')$ , satisfying the symmetry and normalization conditions, gives the product size distribution for binary breakage through the probability of formation of particles with volume v from the breakage of particles of volume v'. The consistency conditions can be written as

$$n(v, 0) \ge 0,$$
  

$$0 \le C(v, v') = C(v', v),$$
  

$$\int_{0}^{v'} \Omega(v, v') dv = 1,$$
  

$$2 \int_{0}^{v'} \Omega(v, v') v dv = v'.$$
(2)

Furthermore, eq. (1) is subject to the following initial conditions:

$$n(v,0) = N(0)\frac{N(0)}{V}\exp\left(\frac{N(0)}{V}v\right)$$
(3)

and

$$n(v,0) = N(0) \left[ 2\frac{N(0)}{V} \right]^2 v \exp\left(-2\frac{N(0)}{V}v\right).$$
(4)

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The analytical solution proposed by the LPA formulation is only valid when the total number of particles is constant with respect to time, although in reality the PSD continuously changes with time. The following kernels are assumed to satisfy the constraints given in LPA formulation:

$$C(v, v') = C,$$
  

$$S(v) = Sv,$$
  

$$\Omega(v, v') = \frac{1}{v'}.$$
(5)

Based on the LPA solution, McCoy and Madras [19] derived the so-called more general analytical solution for the PBE with simultaneous aggregation and breakage. They claim that their analytical solution is applicable for the more general case where the number of particles is not constant, and thus when breakage and aggregation rates are not equal. Thus it represents a more general reversible case, where either aggregation or breakage can dominate. Next to the assumptions made in eq. (5), C is considered to be equal to unity and satisfy the normalization condition both in terms of initial total number of particles and total volume of particles. Equation (1) can be simplified to

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2} \int_0^v n(v',t) n(v-v',t) dv' - n(v,t) \int_0^\infty n(v',t) dv' + 2S \int_v^\infty n(v',t) dv' - Svn(v,t)$$
(6)

and the analytical solution is given by McCoy and Madras [19]:

$$n(v,t) = [\Phi(t)]^2 \exp[-v\Phi(t)],$$
(7a)

where

$$\Phi(t) = \Phi(\infty) \frac{1 + \Phi(\infty) \tanh(\Phi(\infty) (t/2))}{\Phi(\infty) + \tanh(\Phi(\infty) (t/2))}$$

and

$$\Phi\left(\infty\right) = \sqrt{2S}.\tag{7b}$$

The parameter  $\Phi(\infty)$  allows defining the relative weight between breakage and aggregation S/C, by choosing suitable values of the breakage constant S and the aggregation constant C. Setting t = 0 in eq. (7b) and inserting the value of  $\Phi(t)$  in eq. (7a), the initial conditon, for any value of S, becomes

$$n(v, 0) = \exp(-v)$$
. (8)

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Investigating the analytical solution mentioned above in particular, and the related works of McCoy and Madras [19], Lage [22] and Patil and Andrews [23] in general, one can make the following remarks:

*Remark* 1. The so-called analytical solution in eqs (7a) and (7b) is the conversion of the solution derived by Patil and Andrews [23]. Note that eq. (7) in McCoy and Madras [19] naturally satisfies the initial conditions (eq. (6)) which is similar to the solution suggested by Patil and Andrews [23].

*Remark* 2. Therefore, the so-called analytical solution in eqs (7a) and (7b) has no closed-form solution for the initial conditions (3) and (4) as expected.

*Remark* 3. McCoy and Madras [19] overcame this drawback by replacing  $\Phi(t)$  with  $\Phi(\infty)$  in eq. (7a) to obtain long-time asymptotic solution for initial conditons given by eqs (3) and (4) (for example, see eq. (12) in the same paper).

In the following section, we adapt the analytical solution obtained by Pinar and Öziş [20,21] to find the solution of the batch PBE problem considered.

## 3. The auxiliary equation method approach

The auxiliary equation method (AEM) suggested recently by Pinar and Özis [20,21] has been successfully applied in nonlinear physical models to develop new analytical solutions with appropriately chosen parameters. In this paper, we expand the methodology to a batch PBE which is inherently a nonlinear partial integrodifferential equation within a mathematical framework. The detailed features of this method can be read from Pinar and  $\ddot{O}_{2is}$  [20,21]. However, for the sake of brevity, the adjustment of the analytical method for the proposed solution is mentioned. In the previous section, the batch PBE is introduced briefly. For the problem considered in this paper, it is worth mentioning that the time coordinate has a more dominating role. This means that the proposed analytical solution should essentially be time-dependent (transient) with other physical parameters. Transient solutions are characterized by distributions that evolve over several orders of magnitude in volume, often through very steep fronts, before converging to a final steady-state [24]. Therefore, the proposed analytical solution should also hold the vessel volume v at time t in the volume range (v, v + dv) as an effective parameter to make the simulation more realistic. But the particle size distribution is defined so that n(v, t) dx is the number of particles per vessel volume at time t in the volume range (v, v + dv). Therefore, the total volume =  $\int_0^{+\infty} n(v, t)v \, dv$  must also be conserved.

Following the methodology in Pinar and Öziş [20,21], the nonlinear partial integrodifferential population balance equation can be readily reduced to

$$\frac{\partial^2 n\left(\zeta\right)}{\partial \zeta^2} = \frac{1}{2} \int_0^{\zeta} n(\zeta') \frac{\partial n(\zeta-\zeta')}{\partial \zeta} d\zeta' + \frac{1}{2} n(\zeta) - \frac{\partial n\left(\zeta\right)}{\partial \zeta} \int_0^{\zeta} n(\zeta') d\zeta' - n^2(\zeta) - 3Sn(\zeta) - Sv \frac{\partial n(\zeta)}{\partial \zeta}$$
(9)

ordinary integrodifferential equation in independent single variable  $\zeta$  where  $\zeta = \zeta(v, t)$  is a function of particle volume v and the time t. Consequently, the original eq. (1) and the complementary eq. (9) are invariant under the appropriate transformation  $\zeta = \zeta(v, t)$  and also their solutions.

To solve eq. (9) using the solution ansatz (see eq. (3) in Pinar and Öziş [20]) and balancing the nonlinear term with the formula given in the same paper, one can easily determine the solution series as a second-order polynomial

$$u(\zeta) = g_0 + g_1 z(\zeta) + g_2 z^2(\zeta) \tag{10}$$

in  $z(\zeta)$  and the coefficients  $g_0$ ,  $g_1$  and  $g_2$ , the free parameters, can be further determined. By means of balancing, one ensures that the order of the polynomial (eq. (10)) is optimized in such a way that this polynomial spans the solution space entirely, namely, the obtained solution is in closed form (i.e. exact solution) and there is no need to use higherorder polynomials. It is because, as underlined above, the obtained solution is already an exact one.

Referring to the initial condition, which is in the form of an exponential distribution, the expected solution is therefore always exponential. Hence, the auxiliary equation (Case 6 in Table 1 of Pinar and Öziş [20] is selected) is expressed as

$$\left(\frac{\mathrm{d}z}{\mathrm{d}\zeta}\right)^2 = a_2 z^2(\zeta) + a_6 z^6(\zeta) \tag{11}$$

with the solution

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$$z(\zeta) = e^{\left(-\frac{1}{4}\text{LambertW}\left(-\frac{1a_{6}e^{(4\sqrt{a_{2}}(-\zeta+-CI))}}{2a_{2}}\right) - \sqrt{a_{2}}(\zeta--CI)\right)}$$
(12)

which behaves in an exponential form. Hence using the methodology in Pinar and Öziş [20], the parametric general solution of the PBE reads as

$$n(v,t) = \frac{-3s}{2} + g_1 e^{\left(-\frac{1}{4}\text{LambertW}\left(\frac{1}{6}\frac{a_6\alpha\mu}{a_6}\left(4\sqrt{-\frac{3S}{a\mu}}(-\alpha v - \mu t + CI\right)\right)}{S}\right) - \sqrt{-\frac{3S}{\alpha\mu}}(-\alpha v - \mu t) + \sqrt{-\frac{3S}{\alpha\mu}}-CI\right)} - \frac{2}{9}\frac{g_1^2 e^{\left(-\frac{1}{4}\text{LambertW}\left(\frac{1}{6}\frac{a_6\alpha\mu}{a_6}\left(4\sqrt{-\frac{3S}{\alpha\mu}}(-\alpha v - \mu t - CI\right)\right)}{S}\right) - \sqrt{-\frac{3S}{\alpha\mu}}(-\alpha v - \mu t) + \sqrt{-\frac{3S}{\alpha\mu}}-CI\right)}{S}}$$
(13)

Using the following case studies, the AEM solution (eq. (13)) will be tested with the aforementioned restrictions.

Case study 1: Predominant aggregation (S = 0.25) For a predominant aggregation condition, the AEM solution can be written in its expanded form as

$$n(v, t) = -\frac{3}{2} + (0.25e^{-4/v} + 0.55)e^{-\frac{1}{4}LambertW(-0.02667(0.01+0.25 \tanh(0.25v))e^{(-13.8564v+3.4641t-3.4641)}) - 3.4641v+0.866t-0.866)} - \frac{2}{9}(-0.25e^{-4/v} + 0.55)^2e^{(-\frac{1}{4}LambertW(-0.02667(0.01+0.25 \tanh(0.25v))e^{(-13.8564v+3.4641t-3.4641)}) - 3.4641v+0.866t-0.866))^2},$$
(14)

where the parameters of the general PBE solution (see eq. (13)) are given below:

$$g_1 = -0.25e^{-4/\nu} + 0.55, \quad \alpha = 0.8, \quad \mu = -0.2, \quad \_CI = -0.2,$$
  
 $a_6 = 0.01 + 0.25 \tanh(0.25\nu).$ 

Figure 1 shows the comparison of a particle volume-based number density distribution at time t = 1 for AEM solution (eq. (14)) and the comparison with the analytical solution obtained by McCoy and Madras [19]. It can be clearly seen that for a predominant aggregation (S = 0.25), the proposed solution with restrictions overlaps with the available analytical solution.



**Figure 1.** Comparison of AEM solution with the analytical solution of McCoy and Madras [19] at t = 1 for predominant aggregation S = 0.25.

Case study 2: Balanced aggregation and breakage (S = 0.5)

For a balanced aggregation and breakage, the AEM solution can be written in its expanded form as



where the parameters of the general PBE solution (see eq. (13)) are given below:

$$g_1 = \sqrt{2}e^{(-1/2\nu^2)}, \quad \alpha = 2.96, \quad \mu = -4.912, \quad \_CI = \nu^3 + \nu, \quad a_2 = 10\sqrt{2}\tanh\left(\frac{\sqrt{2}}{2}\nu\right), \quad a_6 = 15 + 5\sqrt{2}\tanh\left(\frac{\sqrt{2}}{2}\nu\right)$$

The result of the above AEM solution (eq. (15)) and the comparison with the analytical solution obtained by McCoy and Madras [19] are given in figure 2.

Case study 3: Predominant breakage (S = 1.0)

For a predominant breakage condition, the AEM solution can be written in its expanded form as



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where the parameters of the general PBE solution (see eq. (13)) are given below:

$$g_{1} = \sqrt{2}e^{\left(-(\sqrt{2}/2v^{2})-4\right)^{2}} + 1.2, \quad \alpha = 0.6, \quad \mu = -3.5, \quad \_CI = v - 2$$
$$a_{2} = 10\sqrt{2}\tanh\left(\frac{\sqrt{2}}{2}v\right), \quad a_{6} = 15 + 5\sqrt{2}\tanh\left(\frac{\sqrt{2}}{2}v\right).$$

Figure 3 shows the comparison of the AEM solution (eq. (16)) with the analytical solution obtained by McCoy and Madras [19]. As can be seen from both figures 2 and 3, the AEM solutions expectedly preserve the general trend of the exponential distribution form with the analytical solutions presented in [19]. The minor deviations observed might be due to the basic assumptions (i.e. the method of transformation in auxiliary equation approach) that was made beforehand in the construction of the analytical solutions presented in this paper, as compared to the LPA formulation used [19,22,23].

## 4. Results and discussions

It is important to note that a population balance equation is analogous to a mass balance equation, solved in terms of moments. The PBE describes a balance law for the number of individuals of a population. What makes PBEs more attractive than the ordinary mass balance equations is the continuous change in population and the several mechanisms that occur within the same control volume. Owing to several particulate phenomena, descriptions of the dynamic behaviour of particulate processes involve specifying the temporal



Figure 2. Comparison of AEM solution with the analytical solution of McCoy and Madras [19] at t = 1 for balanced aggregation and breakage S = 0.5.

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Figure 3. Comparison of AEM solution with the analytical solution of McCoy and Madras [19] at t = 1 for predominant breakage S = 0.1.

change in the distribution of properties of the particle. This distribution is a part of the state of the system. Thus particulate processes are inherently distributed parameter systems and the choice of these parameter(s) plays a dominant role in the temporal change of the particle. In the framework of population balances, the state of an individual particle is represented by a particle state vector containing external coordinates, such as the position of a particle in physical space, namely time and internal coordinates representing the particle properties, i.e., particle size/volume. Therefore, a 'well-defined' analytical solution for particle size distribution (PSD) must possess these two dominant variables – time t and particle volume v in the volume range (v, v + dv) – explicitly in their exact solutions along with other consequential parameters to make correct amendments. In figure 1, the analytical solution proposed using AEM with the aforementioned restrictions overlaps with the analytical solution found in [19] because in predominant aggregation (S = 0.25), the effect of the particle volume is insignificant and the AEM solution is dominated only by time t which is why the solution completely overlaps with the available analytical solution. For figures 2 and 3, i.e., balanced aggregation and breakage (S = 0.5) and predominant breakage (S = 1.0), the effect of particle volume is predominant in our solutions due to the presumption of the derivation of the analytical solution whereas the effect of volume in the analytical solution proposed by McCoy and Madras [19] is subsidiary. This fundamental difference explains the slight variation between the two solutions, and based on the assumptions proposed earlier, a more realistic representation of the solutions is obtained compared to the analytical solution proposed by McCoy and Madras [19] for the problem considered.

In this study, the proposed analytical solutions have been constructed on two leading parameters t and v, so that at any time t, there is a distribution with a function of v. This is because, as mentioned earlier, the population of particles is characterized by its particle property distribution, which is described mathematically by a number density function which in this case depends on  $\zeta = \zeta(v, t)$  and is a function of time t and volume v, while  $\zeta$  may be taken as a state vector in general. It is believed that this function represents the (average) number of particles per volume of particle state space more correctly. It is assumed that the deterministic approach is reasonable only if large populations are considered. It is also further assumed that the number density function is sufficiently smooth to be differentiated with respect to its arguments. This is why the actual number of particles in a certain area of the particle state space is determined by the integral of the number density function over this area, and it is this phenomenon that distinguishes the analytical solution from spatially distributed systems. Indeed in McCoy and Madras [19], the solution is given in terms of moments, and for this reason it is not possible to see explicitly the effect of the particle volume v appearing in the analytical solution. Also, as for these moments, there is no exact way to get back to the original distribution from these moments. This is because when the moments of distribution are considered, average properties such as the total number, total volume, etc. can only be obtained which might cause a loss in information about the details of the distribution [25,26]. Moreover, our solution function (eq. ((13))) is clearly an exponential function (fully analytical expression) to the base e. Hence the solution function has domain  $(-\infty, \infty)$  and the range of the solution is  $(0, \infty)$  which preserves all the mathematical and physical properties of the batch PBE model as expected, whereas analytical solution proposed by McCoy and Madras [19] artificially expand the solution domain as pointed out in Remark 3 in the paper.

# 5. Conclusions

In this paper, an effective analytical simulation technique is proposed to solve batch PBE involving particulate aggregation and breakage by making use of appropriate solution(s) of associated complementary equation via AEM. Travelling wave solutions of the complementary equation of nonlinear partial integrodifferential equation with appropriately chosen parameters is taken to be analogous to the description of the dynamic behaviour of the particulate processes of a PBE. Hence, using suitably chosen parameters, the analytical solution proposed in this paper reproduces the expected behaviour of the problem and is compatible with the analytical solution available in literature. In addition, the present approach is flexible, and thereby more efficient than the analytical approach obtained in the literature.

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