The Adomian decomposition method for Solving Batch Crystallization Models

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***Abstract*—A new semi analytic method is proposed for solving population balance equations (PBE). The PBE include the kinetic processes of nucleation, growth, aggregation and breakage.**

The growth and aggregation attained high interest in chemical engineering and the dynamic behavior of crystals size distributions and in this finally their utility the solutions should be helpful in describing the dynamic behavior of any particulate system in which aggregation and growth are taking place.

The results obtained in all cases show that the predicted particle size distributions converge exactly in a continuous form to that of the analytical solutions

Keywords*— *crystals; population balance equations; aggregation; growth; breakage .

I. Introduction

Crystallization is the process of solid formation in the form of crystals from a homogeneous solution. It is a solid-liquid separation technique in which the solute mass transfers from the liquid solution to a pure solid crystalline phase. The process is suitable for separations and puriflcations in pharmaceutical, chemical and food industries. For example, it is used in petro-chemical industry for separation and puriflcation of hydrocarbons, for manufacturing of polymers, and for the production of high valued chemicals and house hold products .

Analysis of a particle system desired to synthesize the behavior of the particle population and its environment by the behavior of individual particles in their local environment. It is described by the density of a suitable extensive variable, usually the number of particles, but sometimes (more correctly) by other variables such as mass or volume of particles. usual population balance equations (PBEs) expressing the conservation laws for hardware systems

The population balance equation (PBE) is analogous to the mass and energy balance equations but provides more information to investigate and analyze the problem.

They were introduced in the field of chemical engineering by Hulbert and Katz (1964)[1] and later fully developed by Randolph and Larson (1988)[2]. However, their applications were limited due to a lack of computational power. Since high speed computers are available now, they became popular which is reflected by their use in several areas of chemical and biochemical engineering. PBE is a combination of different phenomena which contribute to the change in particles population.

In a number of diverse engineering fields used population balance equations (PBEs) sush as emulsification, flocculation, crystallization, include polymerization, polymer degradation, aerosol, biological.

The object of this work is to present new technique Ademain decomposition method for solving certain forms of partial integrodifferential equations arising from (ADM) modeling population balances.

The Ademain decomposition method have attained high interest in applied mathematics and chemical engineering, because it allow solution of both linear and nonlinear functional equations without discretizing the equations or approximating the operators by such schemes as linearization or perturbation. The solution, when it exists, is found in the form of a rapidly converging series.

Comparison between the analytic solutions and the semi-analytique solutions that obetained by Ademain's method indicates it can be accurately predicted by the proposed

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method. In addition, the proposed method is easy to implement with few computational requirements.

II. THE POPULATION BLANCE EQUATIONS

In general, the population balance equation (PBE) is a wellestablished equation for describing the evolution of the dispersed phase. It represents the net rate of number of particles that are formed by breakage, aggregation, growth and could be written for a flow into a well-stirred vessel as [1-2] :

$$\frac{\partial n(l,t)}{\partial t}+\frac{\partial[Gn(l,t)]}{\partial l} = Q_{nuc}-n(l,t)\int_0^\infty \omega(l,l')n(l',t)dl' + \int_l^\infty \beta(l/l')\Gamma(l')n(l',t)dl' - \Gamma(l)n(l,t) + \frac{l^2}{2}\int_0^l \frac{\omega((l^3-l'^3)^{1/3},l')n(l',t)n((l^3-l'^3)^{1/3},t)dl'}{(l^3-l'^3)^{2/3}} \quad (1)$$

III. THE ADOMIAN DECOMPOSITION METHOD

Since the 1980s, Adomian proposed a new and ingenious method for exactly solving nonlinear functional equations [3]. The method has been applied to many frontier problems in engineering, physics, biology and chemistry among other fields [4]. The Adomian decomposition method (ADM) gives the solution as an infinite series usually converging to an accurate solution [5].

The general form of a differential equation be

$$Fu=g. \quad (2)$$

$$F=L+R+N. \quad (3)$$

(3) into (4) become

$$Lu+Ru+N=g. \quad (4)$$

Where L is easily invertible operator, R is the remainder of the linear operator and N corresponds to the non-linear terms.
We can write (4)

$$Lu=g-Ru-Nu. \quad (5)$$

Multiple (5) by L^{-1} be

$$L^{-1}(Lu)=L^{-1}g-L^{-1}(Ru)-L^{-1}(Nu). \quad (6)$$

Where $L^{-1}=\int \ldots \int(.)(dt)^n$ is the inverse of operator L.

So (6) become

$$u=u_0-L^{-1}(Ru)-L^{-1}(Ru). \quad (7)$$

Therefore, u can be presented as a series

$$u(x)=\sum_{n=0}^{\infty}u_n. \quad (8)$$

The non-linear term *N (u)* will be decomposed by the infinite series of Adomian Polynomials A_n[6]

$$Nu=\sum_n^\infty A_n. \quad (9)$$

$$A_n=\frac{1}{n!}\frac{d^n}{d\lambda^n}\left[N\left(\sum_{i=0}^\infty \lambda^i u_i\right)\right]_{\lambda=0} \quad n=0,1,2,.. \quad (10)$$

Y. Cherruault and al [7] has been studied the convergence of the Adomian decomposition.

IV. RESULTS AND DISCUSSION

1. Aggregation

A general description of aggregation with respect to length in any system can be expressed as follows[8], but with different aggregation kernels

$$\frac{\partial n(l,t)}{\partial t}=\frac{l^2}{2}\int_0^l \frac{\omega((l^3-l'^3)^{1/3},l')n(l',t)n((l^3-l'^3)^{1/3},t)dl'}{(l^3-l'^3)^{2/3}} - n(l,t)\int_0^\infty \omega(l,l')n(l',t)dl'. \quad (11)$$

1.1 Constant aggregation kernel

A constant aggregation kernel was adopted,

$$\omega(l,l')=C. \quad (12)$$

In this case the initial condition at $t=0$ is the exponential particle size distribution is given by:

$$n(l,0)=\frac{3N_0}{l_0}l^2 exp\left(\frac{-l^3}{l_0}\right). \quad (13)$$

Where $l_0=N_0=1$.

The solution by the ADM recursion scheme is given by:

$$n_1(l,t)=\frac{1}{4}Cte^{-l^3}l^5\left(l^6-12\right) \quad (14)$$

$$n_2(l,t)=\frac{1}{160}C^2t^2e^{-l^3}l^5\left(l^{12}-60l^6+360\right) \quad (15)$$

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$$n_3(l,t)=\frac{C^3t^3e^{-l^3}l^5\left(l^{18}-168l^{12}+5040l^6-20160\right)}{13440}. \tag{16}$$

Similarly,we can compute $n_4(l,t), n_5(l,t),\ldots,n_m(l,t)$.

Ingeneral $n_m(l,t)$ is the solution of

$$\frac{\partial n_{m+1}(l,t)}{\partial t}=\int_0^t\left(\frac{l^2}{2}\int_0^l\frac{\omega((l^3-l'^3)^{1/3},l')n_m(l',t)n_m((l^3-l'^3)^{1/3},t)dl'}{(l^3-l'^3)^{2/3}}\right)dt$$
$$-\int_0^t\left(n_m(l,t)\int_0^\infty\omega(l,l')n_m(l',t)dl'\right)dt. \tag{17}$$

Hence we calculate the general term as:

$$n_m(l,t)=\frac{3e^{-l^3}l^2\left(1-\frac{Ct}{Ct+2}\right)^2 l^{3(2m-1)}(Ct)^m(Ct+2)^{-m}}{\sqrt{\frac{Ct}{Ct+2}}^{\,2}\,\Gamma(2m)}. \tag{18}$$

Then

$$n(l,t)=\sum_{m=0}^{\infty}n_m(l,t)=\frac{12e^{-l^3}l^2\sinh\left(\frac{\sqrt{C}\sqrt{t}l^3}{\sqrt{Ct+2}}\right)}{\sqrt{C}\sqrt{t}(Ct+2)^{3/2}}), \tag{19}$$

which converges to the exact solution.

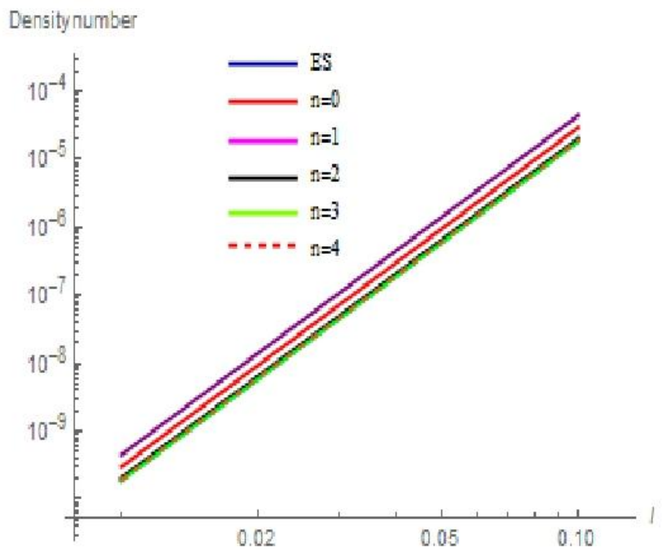

Fig. 1: The effect of the truncation of the series on the solution using $n=$ 0 to 4 iterations and $C=1$, using the exact solution as given by eq.(19) (ES continuous line) for the case of constant aggregation kernel

1.2 Sum aggregation kernel

we use a sum kernel of the form $\omega(l,l')=B_0(l^3+l'^3)$ where l and l' are the sizes of particles and $B_0=1$. The initial particle size distribution is the same as given by equation (13)

The solution using the ADM is derived as follows:

$$n_0(l,t)=3l^2e^{-l^3} \tag{20}$$

$$\frac{\partial n_{m+1}(l,t)}{\partial t}=\int_0^t\left(\frac{l^2}{2}\int_0^l\frac{\omega((l^3-l'^3)^{1/3},l')n_m(l',t)n_m((l^3-l'^3)^{1/3},t)dl'}{(l^3-l'^3)^{2/3}}\right)dt$$
$$-\int_0^t\left(n_m(l,t)\int_0^\infty\omega(l,l')n_m(l',t)dl'\right)dt. \tag{21}$$

From which we calculate the solutions components

$$n_1(l,t)=\frac{3}{2}B_0te^{-l^3}l^2\left(l^6-2l^3-2\right). \tag{22}$$

$$n_2(l,t)=\frac{1}{4}B_0^2t^2e^{-l^3}l^2\left(l^{12}-6l^9-3l^6+18l^3+6\right). \tag{23}$$

$$n_3(l,t)=\frac{1}{48}B_0^3t^3e^{-l^3}l^2\left(l^{18}-12l^{15}+12l^{12}+120l^9-60l^6-168l^3-24\right). \tag{24}$$

$$n_m(l,t)=3l^2e^{-B_0t}e^{l^3\left(-\left(2-e^{-B_0t}\right)\right)}\sum_{m=0}^{\infty}\frac{\left(l^3\right)^{2m}\left(1-e^{-B_0t}\right)^m}{(m+1)!\Gamma(m+1)}. \tag{25}$$

Using the above general term, the general summation is given by:

$$n(l,t)=\sum_{m=0}^{\infty}n_m(l,t)=\frac{3e^{l^3\left(e^{-B_0t}-2\right)-\frac{-B_0t}{2}}I_1\left(2e^{-\frac{1}{2}(-B_0t)}\sqrt{-1+e^{-B_0t}}\,l^3\right)}{l\sqrt{e^{-B_0t}-1}}. \tag{26}$$

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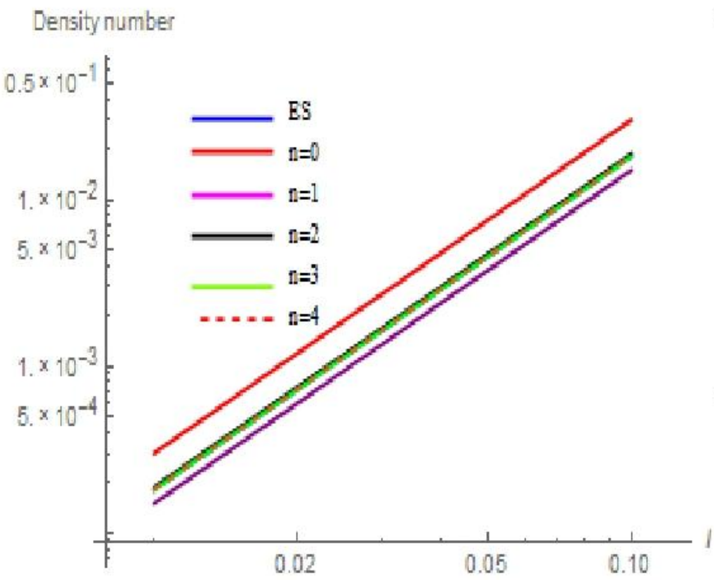

Fig. 2: The effect of the truncation of the series on the solution using $n=$ 0 to 4 iterations and $B_0 = 1$, using the exact solution as given by eq.(26) (ES continuous line) for the case of sum aggregation kernel

1.3 Product aggregation kernel

The product aggregation kernel is given by $\omega(l,l') = B_0(l^3 l'^3)$, where $B_0 = 1$. The initial distribution is the same as given by equation (13) The Adomian recursion scheme is given by:

$$n_0(l,t) = 3e^{-l^3} l^2. \quad (27)$$

$$\frac{\partial n_{m+1}(l,t)}{\partial t} = \int_0^t \left(\frac{l^2}{2} \int_0^l \frac{\omega((l^3 - l'^3)^{1/3}, l') n_m(l',t) n_m((l^3 - l'^3)^{1/3}}{(l^3 - l'^3)^{2/3}} - \int_0^t \left(n_m(l,t) \int_0^\infty \omega(l,l') n_m(l',t) \mathrm{d}l' \right) dt. \quad (28)$$

$$n_1(l,t) = \frac{1}{4} B_0 t e^{-l^3} l^5 (l^6 - 12) \quad (29)$$

$$n_2(l,t) = \frac{1}{240} B_0^2 t^2 e^{-l^3} l^8 (l^{12} - 60 l^6 + 360) \quad (30)$$

$$n_3(l,t) = \frac{B_0^3 t^3 e^{-l^3} l^{11} (l^{18} - 168 l^{12} + 5040 l^6 - 20160)}{40320}. \quad (31)$$

Using the above terms, the general term is deduced as:

$$n_m(l,t) = 3l^2 e^{l^3(-(B_0 t + 1))} \left(\frac{\sqrt{\pi}\, 2^{-2m-1} (B_0 t l^9)^m}{m! \left(m + \frac{1}{2} \right)! (m+1)!} \right). \quad (32)$$

And the closed summation can be written as:

$$n_m(l,t) = \sum_{m=0}^{\infty} 3l^2 e^{l^3(-(B_0 t + 1))} \left(\frac{\sqrt{\pi}\, 2^{-2m-1} (B_0 t l^9)^m}{m! \left(m + \frac{1}{2} \right)! (m+1)!} \right). \quad (33)$$

Finally, this summation is reduced to:

$$n(l,t) = 3l^2 e^{-B_0 t l^3 - l^3} F\left(\{\ \}, \left\{ \frac{3}{2}, 2 \right\}, \frac{1}{4} B_0 t l^9 \right). \quad (34)$$

Where F is the hypergeometric function.

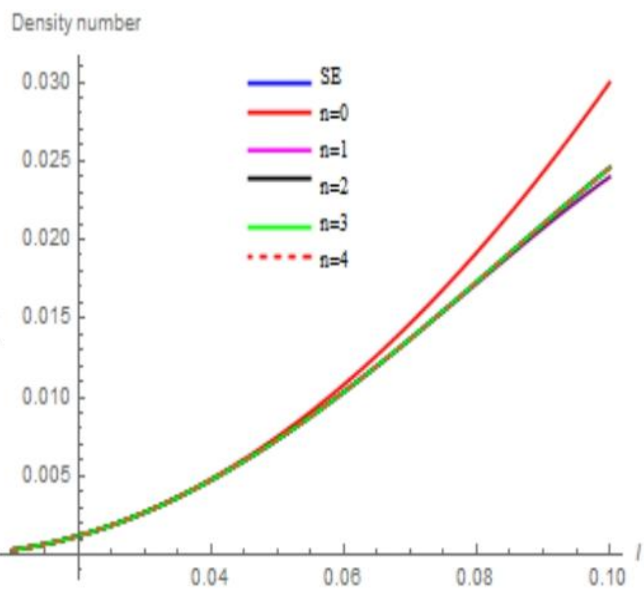

Fig. 3: The effect of the truncation of the series on the solution using $n=$ 0 to 4 iterations and $B_0 = 1$, using the exact solution as given by eq.(34) (ES continuous line) for the case of product aggregation kernel

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2. Growth

A general description of growth with respect to length in any system can be expressed as follows:

$$\frac{\partial n(l,t)}{\partial t}+\frac{\partial[Gn(l,t)]}{\partial l}=0. \quad (35)$$

linear growth rate. For the diffusion-controlled growth, the growth rate can be expressed as[4]

$$G(l,t)=\frac{a}{l}. \quad (36)$$

With the initial condition is the same as given by equation (13). We applied the ADM on the equation (36) can be written as:

$$n(l,t)=-\int_0^t\left(\frac{\partial[Gn(l,t)]}{\partial l}\right)dt. \quad (37)$$

We find the solution to Equation (37) by the ADM as follows:

$$n_0(l,t)=3l^2e^{-l^3}. \quad (38)$$

$$n_1(l,t)=9ate^{-l^3}l^3-3ate^{-l^3}. \quad (39)$$

$$n_2(l,t)=-\frac{27}{2}a^2t^2e^{-l^3}l+\frac{27}{2}a^2t^2e^{-l^3}l^4-\frac{3a^2t^2e^{-l^3}}{2l^2}. \quad (40)$$

$$n_3(l,t)=-\frac{3a^3t^3e^{-l^3}}{2l}+\frac{27}{2}a^3t^3e^{-l^3}l^5-\frac{3a^3t^3e^{-l^3}}{2l^4}-27a^3t^3e^{-l^3}l^2. \quad (41)$$

Hence, we calculate the general term as:

$$n_m(l,t)=3e^{-\left(l^2-2at\right)^{3/2}}\left(\frac{l\binom{\frac{1}{2}}{m}\left(l^2\right)^{\frac{1}{2}-m}(-at)^m}{l^3}\right). \quad (42)$$

Then

$$n(l,t)=\sum_{m=0}^{\infty}n_m(l,t)=le^{-\left(l^2-2at\right)}\sqrt{l^2-2at}. \quad (43)$$

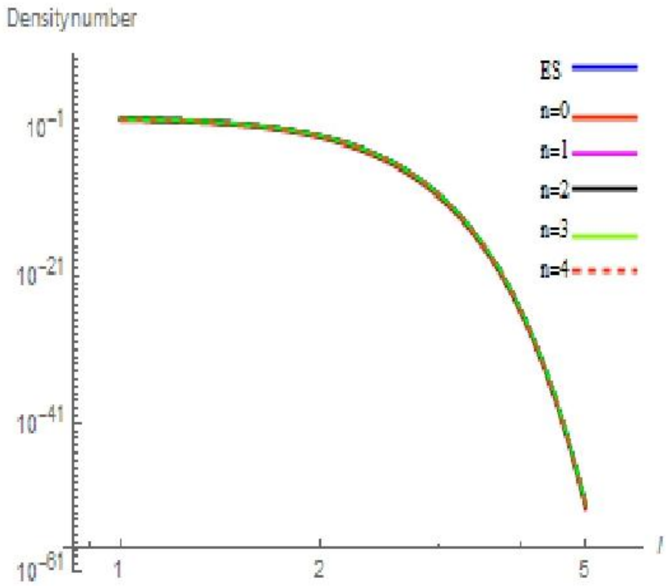

Fig. 4: The effect of the truncation of the series on the solution using $n=$ 0 to 4 iterations and $a=1$, using the exact solution as given by eq.(43) (ES continuous line) for the case of growth

3. Pure breakage

A general description of the breakage process can be written as follows[2]

$$\frac{\partial n(l,t)}{\partial t}=\int_l^{\infty}\beta(l/l')\Gamma(l')n(l',t)\mathrm{d}l'-\Gamma(l)n(l,t). \quad (44)$$

In this case the initial condition at $t=0$ is the exponential particle size distribution:

Where $l_0=N_0=1$.

So $n_0(l,t)=3l^2e^{-l^3}$. (45)

Therefore, the last form of particle breakage, which is suitable for applying the ADM method, is given by:

$$n(l,t)=\int_0^t\left(\int_l^{\infty}\beta(l/l')\Gamma(l')n(l',t)\mathrm{d}l'-\Gamma(l)n(l,t)\right)dt. \quad (46)$$

A power kernel for breakage process

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$$\Gamma(l) = a_0 l^3. \tag{47}$$

And a uniform daughter distribution

$$\beta(l \mid l') = 6l^2/l'^3, 0 \le l \le l' \tag{48}$$

The solution by the ADM recursion scheme is given by:

$$n_1(l,t) = -3ate^{-l^3} l^2 \left(l^3 - 2\right) \tag{49}$$

$$n_2(l,t) = \frac{3}{2} a^2 t^2 e^{-l^3} l^2 \left(l^6 - 4l^3 + 2\right) \tag{50}$$

$$n_3(l,t) = -\frac{1}{2} a^3 t^3 e^{-l^3} l^5 \left(l^6 - 6l^3 + 6\right) \tag{51}$$

$$n_m(l,t) = \frac{(-1)^m \left(3e^{-l^3} a^m t^m \left(\left(l^3 - m\right)^2 - m\right)\right)}{(m+1)!} - 3ate^{-l^3}\left(l^3 - 2\right)l^2 + 3e^{-l^3} l^2. \tag{52}$$

the exact solution is given by summation the above general term and simplified to:

$$n(l,t) = \sum_0^\infty n_m(l,t) = 3e^{l^3(-(at+1))}(atl + l)^2. \tag{53}$$

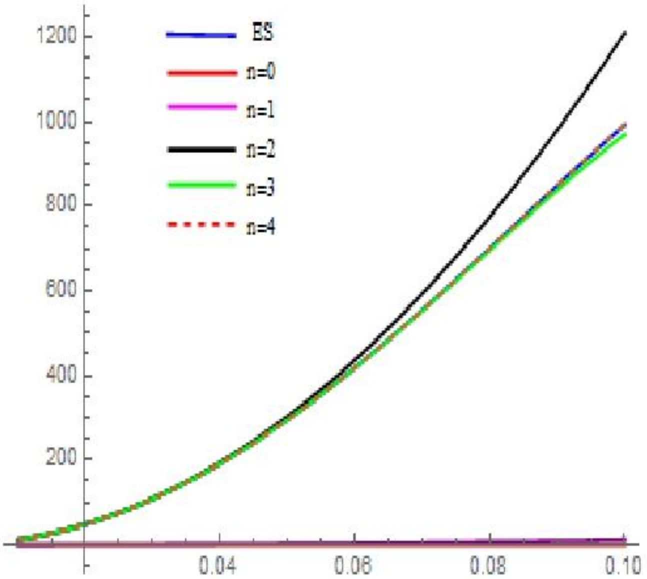

Figure 1: The effect of the truncation of the series on the solution using $n = 0$ to 4 iterations and $a = 1$, using the exact solution as given by eq.(53) (ES continuous line) for the case of pure breakage

V. CONCLUSIONS

The solutions obtained by the ADM technique was infinite power series with appropriate initial conditions.

The Adomain method is able to accurately predict the solution of PBE involving any combination of particle system process, that is, growth and aggregation. The proposed approach is free from stability and dispersion problems of other numerical methods such as the discretization.

The Adomian decomposition method was employed successfully for solving the particle population balance equations in batch crystallization models describing crystals size-dependent aggregation growth, and breakag,.

The solutions obtained by the ADM technique was infinite power series with appropriate initial conditions. The method was found to produce good approximations to the exact solutions with their rapidly converging series for all the cases studied in this work.

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