Thai Journal of Mathematics
Volume 20 Number 2 (2022)
Pages 545–555

http://thaijmath.in.cmu.ac.th

ISSN 1686-0209

Semi-Analytical Solutions of Batch System Population Balance Models

Zehra Pinar

Tekirdağ Namık Kemal University, Faculty of Arts and Science, Department of Mathematics, 59030 Merkez-Tekirdağ, Turkey
e-mail : zpinar@nku.edu.tr

Abstract We propose a semi-analytical method to solve partial integro-differential equations with initial/boundary conditions. This work investigates the semi-analytical solutions of the population balance models (PBMs) for the batch systems. The comparison of obtained solutions with the known exact solutions is given to show the effectiveness of the proposed method. The proposed method is very useful, reliable, and flexible; also, the solutions can play key role population balance models in engineering and science which are different kinds of partial integro-differential equations.

MSC: 49K35; 47H10; 20M12

Keywords: population balance model; batch systems; droplet breakup; semi-analytical solutions

Submission date: 17.06.2019 / Acceptance date: 18.01.2022

1. Introduction

Analytical or semi-analytical solutions are important in many branches of engineering and physics because of singularities, nonlinearities, inhomogeneity and some general initial boundary conditions. Hence, applied mathematicians, engineers and physicists are forced to find analytical or semi-analytical solutions of the problems in hand. Numerous numerical methods have been developed/improved to solve PBM containing whethertime-dependent or time-independent formulations [22, 23, 25]. Among them include the finite difference, finite volume and the finite element approaches (see Ramkrishna [27] for an overview) and several papers have been published till date [1–3]. Many other techniques that can be used to solve Population Balance Equations (PBEs) are the method of moments in which the PBE is solved for moments of the Particle Size Distribution (PSD) [7, 9, 18–20]. The general idea of analytical or semi-analytical solutions depends on various series either asymptotic series or power series. The difference between the series affects the convergence. Therefore, in recent years, there are some novel methods based on integral expansion of the solution before the asymptotic expansion that is based on homotopy theory. Although, all these methods are known, let us briefly mention the methodology given in [4, 10, 13–17, 21, 24, 28]. In addition to these methods, one of

Published by The Mathematical Association of Thailand.

the serial-based methods is the Adomian decomposition method (ADM) that a nonlinear operator expands into a sequence and the terms are repeatedly calculated using Adomian polynomials [8]. From the general view of known analytical and semi-analytical method,we proposed new and basic method. The novel proposed iteration method is also expansion of the semi-analytical method for integral-differential equations proposed by Kheybari [11, 12]. Now, for the aforementioned methods: consider a general nonlinear partial integro-differential equation

$$\frac{\partial^n u}{\partial t^n} + \frac{\partial^n u}{\partial v^n} = F(v, t, u_v, u_t, \ldots, (\kappa_1 u)(v, t), (\kappa_2 u)(v, t), (\kappa_3 u)(v, t)) + f(v, t) \quad (1.1)$$

and $(\kappa_1 u)(v,t) = \int_0^v k_1(v',t)u(v',t)\,dv', (\kappa_2 u)(v,t) = \int_0^\infty k_2(v',t)u(v',t)\,dv', (\kappa_3 u)(v,t) = \int_v^\infty k_3(v',t)u(v',t)\,dv'$ where $k_1(v,t), k_2(v,t), k_3(v,t)$ are continuous functions. For the initial/boundary conditions
$\sum_{j=1}^{n_k} a_{jk} u^{r_{jk}}(\xi_{jk}, \tau_{jk}) = d_k, k = 1, \ldots, n, r_{jk} \in \{1, \ldots, n-1\}$.

The first iteration is obtained as the solution of the linear homogeneous initial/boundary value problem $\frac{\partial^n u_0}{\partial t^n} + \frac{\partial^n u_0}{\partial v^n} = 0$,
$\sum_{j=1}^{n_k} a_{jk} u_0^{r_{jk}}(\xi_{jk}, \tau_{jk}) = d_k, k = 1, \ldots, n, r_{jk} \in \{1, \ldots, n-1\}$.

The general iteration is given as
$\frac{\partial^n u_{i+1}}{\partial t^n} + \frac{\partial^n u_{i+1}}{\partial v^n} = F(v, t, (u_i)_v, (u_i)_t, \ldots, (\kappa_1 u_i)(v, t), (\kappa_2 u_i)(v, t), (\kappa_3 u_i)(v, t)) + f(v, t), i = 0, 1, \ldots, l,$

$\sum_{j=1}^{n_k} a_{jk} u_i^{r_{jk}}(\xi_{jk}, \tau_{jk}) = 0, k = 1, \ldots, n, r_{jk} \in \{1, \ldots, n-1\}$.

To stop the iteration, the classical conditions or the consecutive errors such as absolute error $|u_i - u_{i-1}| < \epsilon$ or relative error $|\frac{u_i - u_{i-1}}{u_i}| < \epsilon$ can be considered that are depending on the successive terms of the iteration.

2. Model Equation

In this part, the semi-analytical solutions of the droplet breakage equation and simultaneous aggregation and breakage problem are obtained by using the novel proposed iteration method. For the model equation, two general cases are considered with three and two sub-cases, respectively. Also, the comparisons with analytical solution (if it is known) and the solutions obtained by ADM will be proposed.

2.1. Breakage Processes in Batch Systems

Breakup with a uniform distribution: It is the possibility of breaking up a particle into two parts, regardless of both the size of the object and the parts. The number-based breakage kernel is independent of v , since it is likely to be of equal size to a given child particle. When a particle is broken, it is assumed that the probability of creating a smaller size particle is equal.

The model is given

$$\frac{\partial n(v,t)}{\partial t} = \int_v^\infty \beta(v,v')S(v')n(v',t)\,dv' - S(v)n(v,t), \tag{2.1}$$

with the initial condition $n(v,0) = e^{-v}$.
The first step is to obtain the initial approximation $\dfrac{\partial n_0(v,t)}{\partial t} + S(v)n_0(v,t), n(v,0) = e^{-v}$.
Then the general steps of the novel proposed iteration method are
$\dfrac{\partial n_i(v,t)}{\partial t} + S(v)n_i(v,t) = \int_v^\infty \beta(v,v')S(v')n_{i-1}(v',t)\,dv', n_i(v,0) = e^{-v}, i = 1,2,\ldots.$
Case 1: The kernels are $\beta(v,v') = \frac{2}{v'}, S(v) = v$ and its analytical solution $n(v,t) = (1+t)^2 e^{-v(1+t)}$ is given by Ziff and McGrady [30].
Now, with the novel proposed iteration method, the semi-analytical solution is obtained and the comparison of the solutions is given by Figure 1.
$n_0(v,t) = e^{-v(1+t)}$,
$n_1(v,t) = (2ln(1+t)+1)e^{-v(1+t)}$,
$n_2(v,t) = (2ln(1+t)^2 + 2ln(1+t)+1)e^{-v(1+t)}$,
$\vdots$

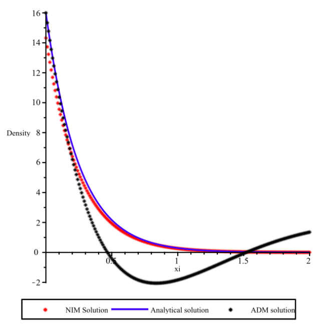
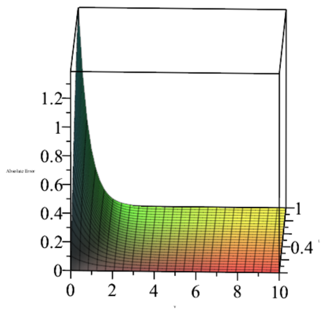


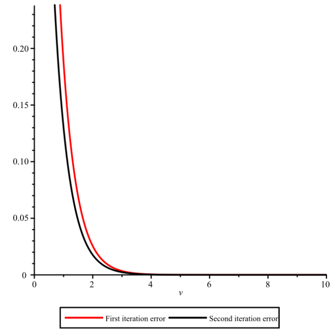
FIGURE 1. The comparison of the solutions is given for $t = 3$.

The novel proposed iteration method converges the analytical solution faster than ADM. So, the second iteration of the novel proposed method gives better result than the third iteration of ADM. Also, the absolute error is zero when $(v,t) \to \infty$,i.e. and $\lim_{(v,t)\to\infty} |u_n - u_{n-1}| = 0$ the error is calculated between the semi-analytical and the known analytical solutions [30], and given by Figure 2.

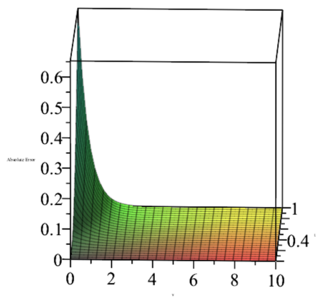
Case 2: The kernels are $\beta(v,v') = \frac{2}{v'}, S(v) = v^2$ and its analytical solution $n(v,t) = (1+2t(1+v))e^{-v(1+tv)}$ is given by Ziff and McGrady [30].
Now, with the novel proposed iteration method, the semi-analytical solution is obtained and the comparison of the solutions is given by Figure 3.
$n_0(v,t) = e^{-vt(1+v)}$,
$n_1(v,t) = (2Ei(1,tv) + \frac{-2e^{-0.001v^2}Ei(1,0.001v)+e^{-v}}{e^{-0.001v^2}})e^{-v^2t}$,



(a) The consecutive error $|u_n - u_{n-1}|$



(b) The consecutive error $|u_n - u_{n-1}|$ for $t = 1$



(c) The pointwise error $|u_{\text{exact}} - u_n|$

FIGURE 2. The error comparisons of the solutions are given.

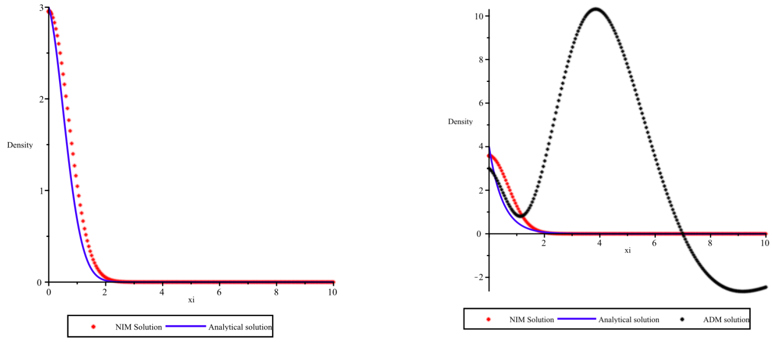
$\vdots$

A parabolic distribution: The kernels are considered as $\beta(v, v') = \frac{24(v^2 - vv') + 6v'^2}{v'^3}$, $S(v) = v$ and the analytical solution is not available to our knowledge.
Now, with the novel proposed iteration method, the semi-analytical solution is obtained and represented by Figure 4.
$n_0(v, t) = e^{-v(1+t)}$,
$n_1(v, t) = (24vt + 6ln(t + 1) + 1)e^{-v(t+1)}$,
$\vdots$

2.2. Breakage Processes in Continuous Systems

The model is

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{\theta}(n^{feed}(v,t) - n(v,t)) + \int_v^{\infty} \beta(v,v')S(v')n(v',t)\,dv' - S(v)n(v,t), \tag{2.2}$$



(a) (b)

FIGURE 3. The comparison of the solutions is given for $t = 3$.

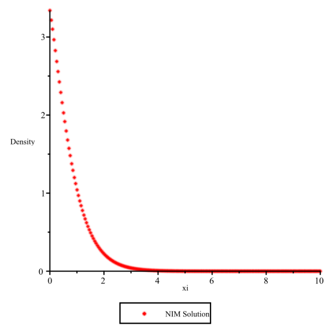


FIGURE 4. The solution is given for $t = 3$.

with the initial condition $n(v, 0) = 0$.
The first step is to obtain the initial approximation
$\dfrac{\partial n_0(v,t)}{\partial t} + (S(v) + \frac{1}{\theta})n_0(v,t) = 0, n_0(v,t) = 0.$
Then the general steps of the novel proposed iteration method are

$$\frac{\partial n_i(v,t)}{\partial t} + (S(v) + \tfrac{1}{\theta})n_i(v,t) = \int_v^\infty \beta(v,v')S(v')n_{i-1}(v',t)\,dv' + \tfrac{n^{feed}(v,t)}{\theta}, n_i(v,t) = 0, i = 1, 2, \ldots. \tag{2.3}$$

The kernels are $\beta(v, v') = \frac{2}{v'}, S(v) = v$ and $n^{feed} = e^{-v}$.
Now, with the novel proposed iteration method, the semi-analytical solution is obtained.
$n_0(v,t) = 0$,
$n_1(v,t) = ae^{-vt}$,
$n_2(v,t) = -\frac{1}{2}at^2e^{-v}(a + v - 1) + ate^{-v}$,

$\vdots$

2.3. Simultaneous Aggregation and Breakage

Regardless of spatial dependence, the party PBE, its growth-based formulation is called LPA and is expressed as follows:

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v C(v',v-v')n(v',t)n(v-v',t)\,dv' - n(v,t)\int_0^\infty C(v,v')n(v',t)\,dv' + 2\int_v^\infty \beta(v,v')S(v')n(v',t)\,dv' - S(v)n(v,t) \tag{2.4}$$

where the $n(v,t)$ is the number density function in terms of the particle volume $v.C(v,v')$,is the aggregation kernel that describes the frequency at which particles with volume v and v' collide to form a particle of volume $v+v'$, $S(v)$ and $\beta(v,v')$ are the breakage function and the breakage kernel, respectively. They satisfy the symmetry and normalization conditions and breakage kernel 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:
$n(v,0)\geq 0$,
$0\leq C(v,v')=C(v',v)$,
$\int_0^{v'}\beta(v,v')\,dv=1$,
$2\int_0^{v'}\beta(v,v')v\,dv=v'$.
Furthermore, the initial conditions are given:
$n(v,0)=N(0)\frac{N(0)}{V}exp(\frac{N(0)}{V}v)$ and $n(v,0)=N(0)(2\frac{N(0)}{V})^2 vexp(-2\frac{N(0)}{V}v)$.
The following kernels are considered
$C(v,v')=C, S(v)=Sv, \beta(v,v')=\frac{1}{v'}$.
Based on the LPA solution, for the PBE with simultaneous aggregation and breakage, a general analytical solution was proposed by McCoy and Madras [22]. 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. The solution of McCoy and Madras [22] is:
$n(v,t)=[\phi(t)]^2\,exp\,[-v\phi(t)]$
where,
$\phi(t)=\phi(\infty)\frac{1+\phi(\infty)tanh(\phi(\infty)\frac{t}{2})}{\phi(\infty)+tanh(\phi(\infty)\frac{t}{2})}$ and $\phi(\infty)=\sqrt{2S}$.
The relative weight between breakage and aggregation S/C with the chosen constant values of S and C is determined by the parameter $\phi(\infty)$. Setting $t=0$ in second condition and substituting the value of $\phi(t)$ in first condition, the initial condition, for any value of S, is obtained:
$n(v,0)=exp(-v)$.

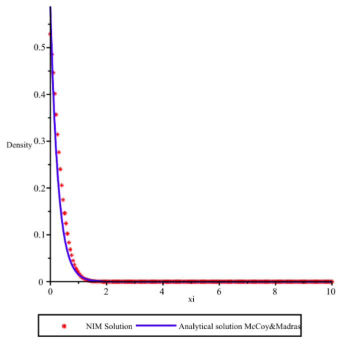
With the novel proposed iteration method, the semi-analytical solution is obtained:

$n_0(v,t)=exp(-v(1+St))$,
$n_1(v,t)=(\frac{vt}{2}+2ln(1+St)+1)exp(-v(1+St))$
$n_2(v,t)=(\frac{7exp(-v)}{2S}v+\frac{exp(-v)}{2S}tv+2exp(-v)ln(1+St)+2\frac{exp(-v)}{S}vln(1+St)^2-3\frac{exp(-v)}{S}v$

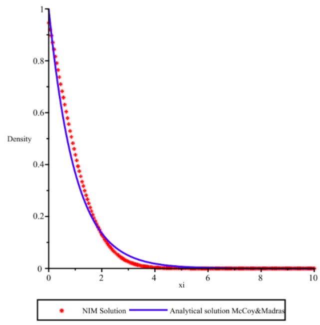
$ln(1+St)+\frac{exp(-v)}{4S}tv^2-\frac{exp(-v)}{4S^2}v^2ln(1+St)-\frac{exp(-v)}{2S^2}vln(1+St)+\frac{exp(-v)}{2S^2}vln(1+St)^2+\frac{exp(-v)}{144S^3}v^3+\frac{exp(-v)}{4S^2}v^2+\frac{exp(-v)}{2S^2}v-\frac{4exp(-v)}{3S}ln(1+St)^3+\frac{exp(-v)}{S(1+St)}+2exp(-v)ln(1+St)^2-2\frac{exp(-v)}{S}(1+St)ln(1+St)^2+\frac{exp(-v)}{144}v^3t^3-\frac{exp(-v)}{S}ln(1+St)tv+\frac{7exp(-v)}{2}vt+2exp(-v)vln(1+St)^2t-2exp(-v)vln(1+St)t+\frac{exp(-v)}{4}v^2ln(1+St)t^2+\frac{exp(-v)}{144}(-504vS^2-v^3-36v^2S-72Sv-144S^2)/S^3)exp(-Svt)$

$\vdots$

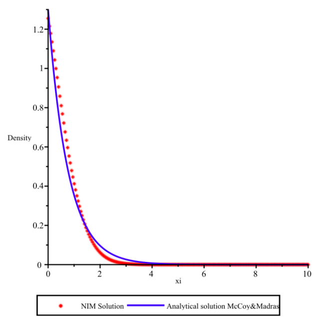
The comparative figures are given for $S=0.25, 0.5, 1$ in Figure 5.



(a) $S=0.25$



(b) $S=0.5$



(c) $S=1$

FIGURE 5. The comparison of the solutions with the given analytical solutions for the considered cases, respectively, for $t=1$.

2.4. Two-dimensional Population Balance Model with Pure Aggregation

The classical one-dimensional PBM does not always properly define the evolution of processes. Therefore, considering the various dimensions and internal shape factors, the use of multidimensional models is necessary and important in terms of compliance with the actual structure. For example, Puel, Fevotte and Klein [26] proposed a two dimensional PBM to simulate crystalline time variations in two internal dimensions and hence the characteristic shape factor (elongation factor the state of rod-like hydroquinone particles). For the well-mixed batch process, bivariate PBM only aggregation term is given

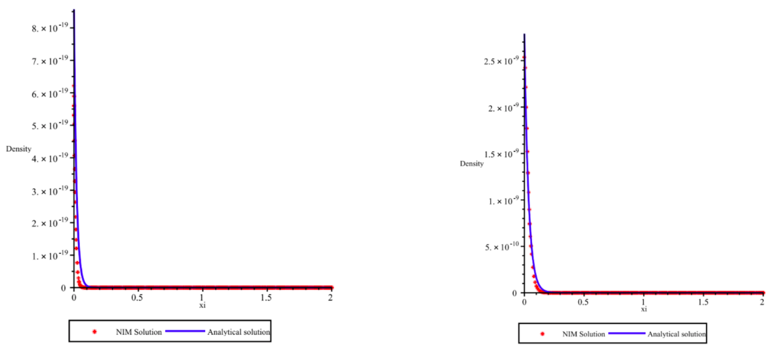
$$\frac{\partial n(t,u,v)}{\partial t} = \frac{1}{2}\int_0^u\int_0^v \beta(t,u-u',v-v',u',v')n(t,u-u',v-v')n(t,u',v')\,du'dv' - \int_0^\infty\int_0^\infty \beta(t,u,v,u',v')n(t,u,v)n(t,u',v')\,du'dv' \tag{2.5}$$

where the initial condition is $n(0,u,v) = n_0(u,v), u,v \in (0,\infty), n(t,u,v)dudv$ is the number of particles presented in the small range $[u,u+du] \times [v,v+dv]$ at any time t,$\beta(t,u,v,u',v')$ is the aggregation kernel that is considered symmetric function. Generally right-hand side of the equation corresponds to aggregation term which includes birth and death terms, in the written order in the equation respectively [29].

Case 1. (Size independent kernel): For this case, the aggregation kernel is considered constant $\beta(t,u,v,u',v') = 1$ and the initial condition is
$n(0,u,v) = \frac{16N_0uv}{m_{10}^2m_{20}^2}exp(-\frac{2u}{m_{10}} - \frac{2v}{m_{20}})$ where $N_0 = 1, m_{10} = m_{20} = 0.04$. Gelbard and Seinfeld [6] proposed the analytical solution.

Case 2. (Size dependent kernel): For this case, the aggregation kernel is considered constant $\beta(t,u,v,u',v') = u+v+u'+v'$ and the initial condition is
$n(0,u,v) = \frac{16N_0uv}{m_{10}^2m_{20}^2}exp(-\frac{2u}{m_{10}} - \frac{2v}{m_{20}})$ where $N_0 = 1, m_{10} = m_{20} = 0.04$. The analytical solution is given by Ferna´ndez-Dı´az and Go´mez-Garcı´a [5].

For the given cases, the semi-analytical solution is obtained via the novel proposed iteration method and compared with given exact solutions.



(a) (b)

Figure 6. The comparison of the solutions with the given analytical solutions for the considered cases, respectively, for $t = 1, v = 1$.

3. Conclusion

Population Balance Model (PBM) is essentially a mesoscale framework for a particulate process that utilizes microscale information and solves using balance equations, essentially non-linear partial differential equations, through efficient implementation of numerical or approximate analytical approaches. In this study, the dynamic behavior of such particulate processes under the effect of aggregation and breakage, in one- and two-dimensions has been studied. Approximate analytical solutions are obtained from the PBE representing the PSD density function by novel proposed iteration method. The novel iteration method looks like Homotopy-based methods and series methods (such as Adomian decomposition method) generate infinite series which convergence uniformly with distinct speeds (of convergence) to the exact solution that can be seen from given figures. This method is straightforward and easy to implement even to two-dimensional integro-differential equations such as in the cases presented in this study. The study also indicates that this approach could be safely implemented to solve complex realistic reactor engineering problems and crystallization problems.

References

[1] A.H. Alexopoulos, A.I. Roussos and C. Kiparissides, Part I: Dynamic evolution of the particle size distribution in particulate processes undergoing combined particle growth and aggregation, Chemical Engineering Science 59 (24) (2004) 5751–5769.

[2] R. Bleck, A fast, approximative method for integrating the stochastic coalescence equation, Journal of Geophysical Research 75 (1970) 5165–5171.

[3] E.G. Chatzi and C. Kiparissides, Dynamic simulation of bimodal drop size distributions in low-coalescence batch dispersion systems, Chemical Engineering Science 47 (2) (1992) 445–456.

[4] A. Dutta, Z. Pinar, D. Constales and T. Ozis, Population balances involving aggregation and breakage through homotopy approaches, International Journal of Chemical Reactor Engineering 16 (6) (2018) 10 pages.

[5] J. Fernández-Díaz, G. Gómez-García, Exact solution of smoluchowski's continuous multicomponent equation with an additive kernel, Europhys Lett 78 (5) (2007) 7 pages.

[6] F. Gelbard and J. Seinfeld, Simulation of multicomponent aerosol dynamics, Journal of Colloid and Interface Science 78 (2) (1980) 485–501.

[7] J. Gimbun, Z.K. Nagy and C.D. Rielly, Simultaneous quadrature method of moments for the solution of population balance equations, using a differential algebraic equation framework, Ind. Eng. Chem. Res. 48 (2009) 7798–7812.

[8] A. Hasseine , A. Bellagoun and H.-J. Bart , Analytical solution of the droplet breakup equation by the Adomian decomposition method, Applied Mathematics and Computation 218 (2011) 2249–2258.

[9] V. Kariwala, Y. Cao and Z.K. Nagy, Automatic differentiation-based quadrature method of moments for solving population balance equations, AIChE Journal 58 (3) (2012) 842–854.

[10] C. Khantree and R. Wangkeeree, Approximate quasi solutions of multiobjective optimization problems, Thai Journal of Mathematics 19 (1) (2021) 221–231.

[11] S. Kheybari, M.T. Darvishi and A.M. Wazwaz, A semi-analytical approach to solve integro-differential equations, Journal of Computational and Applied Mathematics 317 (2017) 17–30.

[12] S. Kheybari, M.T. Darvishi and A.M. Wazwaz, A semi-analytical algorithm to solve systems of integro-differential equations under mixed boundary conditions, Journal of Computational and Applied Mathematics 317 (2017) 72–89.

[13] S.J. Liao, A second-order approximate analytical solution of a simple pendulum by the process analysis method, Journal of Applied Mechanics 59 (1992) 970–975.

[14] S.J. Liao, The Proposed Homotopy Analysis Technique for the Solution of Nonlinear Problems, PhD thesis, Shanghai Jiao Tong University, 1992.

[15] S.J. Liao, An explicit, totally analytic approximation of Blasius' viscous flow problems, International Journal of Non-Linear Mechanics 34 (4) (1999) 759–778.

[16] S.J. Liao, Beyond Perturbation: Introduction to the Homotopy Analysis Method, Boca Raton: Chapman & Hall/ CRC Press, New York, 2003.

[17] S.J. Liao, Homotopy Analysis Method in Nonlinear Differential Equations, Berlin & Beijing: Springer & Higher Education Press, Berlin Heidelberg 2012.

[18] D.L. Marchisio, R.D. Vigil and R.O. Fox, Quadrature method of moments for aggregation-breakage processes, Journal of Colloid and Interface Science 258 (2003) 322–334.

[19] D. L. Marchisio and R.O. Fox, Solution of population balance equations using the direct quadrature method of moments, Journal of Aerosol Science 36 (1) (2005) 43–73.

[20] R. McGraw, Description of aerosol dynamics by the quadrature method of moments, Aerosol Science and Technology 27 (2) (1997) 255–265 .

[21] I. Navarasuchitr, P. Huabsomboon and H. Kaneko, Efficient numerical technique for solving integral equation, Thai Journal of Mathematics 19 (1) (2021) 251–260.

[22] Z. Pınar, A. Dutta, G. Bény and T. Öziş, Analytical solution of population balance equation involving aggregation and breakage in terms of auxiliary equation method, Pramana–Journal of Physics 84 (2015) 9–21.

[23] Z. Pınar, A. Dutta, G. Bény and T.Öziş , Analytical solution of population balance equation involving growth, nucleation and aggregation in terms of auxiliary equation method, Applied Mathematics & Information Sciences 9 (2015) 2467–2475.

[24] Z. Pinar, H. Kocak and Y. Daoud, Semi-analytical solutions of nonlinear equation modelling reaction in a dispersive medium, Karaelmas Science and Engineering Journal 8 (1) (2018) 197–202.

[25] Z. Pinar, Studies on population balance equation involving aggregation and growth terms via symmetries, International Journal of Nonlinear Sciences and Numerical Simulation, 22 (2021) 437–446.

[26] F. Puel, G. Févotte and J. P. Klein, Simulation and analysis of industrial crystallization processes through multidimensional population balance equations. Part 2: a study of semi-batch crystallization, Chemical Engineering Science 58 (2003) 3729–3740.

[27] D. Ramkrishna, Population Balances: Theory and Applications to Particulate Systems in Engineering, Academic Press, San Diego, 2000.

[28] M.S. Rawashdeh and S.Maitama, On finding exact solutions to coupled systems of partial differential equations by the NDM, Thai Journal of Mathematics, 18 (2)

(2021) 607–619.

[29] M. Singh, G. Kaur, T.D. Beer and I. Nopens, Solution of bivariate aggregation population balance equation: a comparative study, Reaction Kinetics, Mechanisms and Catalysis 123 (2018) 385–401.

[30] R.M. Ziff and E.D. McGrady, The kinetics of cluster fragmentation and depolymerisation, Journal of Physics A: Mathematical and General 18 (1985) 3027–3037.