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Original Research Paper

Analytical solutions of the particle breakage equation by the Adomian decomposition and the variational iteration methods

A. Hasseine [a,b,*], Z. Barhoum [a,b], M. Attarakih [c,d], H.-J. Bart [d]

[a] Laboratory LAR-GHYDE, University of Biskra, Algeria
[b] Department of Chemical Engineering, University of Biskra, Algeria
[c] Faculty of Eng. & Tech., Chem. Eng. Dept., The University of Jordan, 11942 Amman, Jordan
[d] Chair of Separation Science and Technology, Center for Mathematical Modeling, Kaiserslautern University, P.O. Box 3049, D-67653 Kaiserslautern, Germany

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ABSTRACT

The breakage in batch and continuous systems has attained high interest in chemical engineering and granulation from a process and from a product quality perspective. The wet granule breakage process in a high shear mixer will influence and may control the final granule size distribution. In this work, we developed analytical solutions of the particle breakage using the population balance equation (PBEs) in batch and continuous flow systems. To allow explicit solutions, we approximate particle breakage mechanisms with assumed functional forms for breakage frequencies. This new framework for solving (PBEs) for batch and continuous flow systems proposed in this work uses the Adomian decomposition method (ADM) and the variational iteration method (VIM). These semi-analytical methods overcome the crucial difficulties of numerical discretization and stability that often characterize previous solutions in of the PBEs. 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 using the two methods.

1. Introduction

Granulation is an important process in a wide range of industries, including agricultural products, detergents, pharmaceutical, food, ore processing, fertiliser and chemical engineering [1,2]. Generally the granulation process is well known as a combination of three rate processes, namely wetting and nucleation, consolidation and growth, breakage and attrition and this is analogous to the process used by chemical engineers in reactor engineering and reactor design [3]. Once these processes are sufficiently understood, then it will be possible to theoretically predict the effect of formulation properties, equipment type and operating conditions on granulation behaviour [4].

The population balance equation is used in a number of diverse engineering fields such as granulation [5–8], crystallization [9,10], fluid bed [11,12], reactors [13,14] the grinding [15], polymerization [16–18], chemical engineering [19,20], emulsification [21], flocculation [22], aerosol [23], biological [24], Process Control [25].

In general, the population balance equation (PBE) is a well-established 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 [26–30]:

$$\frac{\partial n(v,t)}{\partial t}+\frac{\partial[Gn(v,t)]}{\partial v}=\frac{1}{\theta}(n^{feed}(v,t)-n(v,t))+\phi(v,t), \quad (1)$$

where the first term is the rate of accumulation of particle of size v, the second term is the convective flux along the particle internal coordinate with a growth velocity G. The first term on the right hand side is the net bulk flow into the vessel and the second term is the net rate of particle generation by aggregation and breakage and is given by [29–34]:

$$\varphi(v,t)=-\Gamma(v)n(v,t)-\int_0^\infty \omega(v,v')n(v,t)n(v',t)dv' + \int_v^\infty \beta(v/v')\Gamma(v')n(v',t)dv' + \frac{1}{2}\int_0^v \omega(v-v',v')n(v,t)n(v-v',t)dv' + S(v), \quad (2)$$

where $\Gamma(v)$ and $\omega(v,v')$ are the breakage and aggregation frequencies, respectively, and $\beta(v|v')$ dv is the number of daughter particles

* Corresponding author at: Department of Chemical Engineering, University of Biskra, Algeria.
E-mail address: hasseine@yahoo.fr (A. Hasseine).

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Nomenclature

$n(v,t)dv$	number of particles in size range v to v v+dv, at time t
t	Time
$u_m(v,t)$	solution components
v, v'	particle volumes

Greek letters

$\beta(v/v')dv$	fractional number of particles formed in the size range v to $v+dv$ formed upon breakage of particle of volume v'
δ	Dirac delta function
$\Gamma(v')$	number of particles in the size range v to $v+dv$ disappearing per unit time by breakage
θ	residence time
$\omega(v,v')$	aggregation frequency between two particles of volumes v and v'
γ	gamma function
φ	Heaviside Theta

having volume in the range, which are formed upon breakage of a particle of volume v'. The first two terms on the right hand side represent particle loss due to breakup and aggregation succeeded by two terms which represent particle formation due to breakup and aggregation, $S(v)$ is rate at which particles of size v are nucleated.

The objective of this paper is to solve certain forms of the above equation, which is partial integro-differential equation using two new techniques: The Adomian decomposition method and the Variational iteration method. These new techniques have attained high interest in applied mathematics and chemical engineering, because they allow solution of both linear and nonlinear functional equations of various kinds (algebraic, ordinary differential, partial differential, delay differential integral, ...) without discretizing the equations or approximating the operators by such schemes as linearization or perturbation, which changes the physical problem to one that is amenable by prior art. The solution, when it exists, is found in the form of a rapidly converging series such that the time and space coordinates are not discretized.

Of course some problems remain open. For instance, practical convergence of the Adomian decomposition series may be ensured even if the hypotheses of known methods are not satisfied. That means that there still exist opportunities for further theoretical studies of convergence for more general situations. Furthermore, it is not always easy to take into account the boundary conditions for complex domains.

1.1. The Adomian decomposition method

Since the 1980s, Adomian proposed a new and ingenious method for exactly solving nonlinear functional equations [35,36]. The method has been applied to many frontier problems in engineering, physics, biology and chemistry among other fields [30–38]. The Adomian decomposition method (ADM) gives the solution as an infinite series, which usually converges to the exact solution [39].

The general form of a differential equation can be written as

$$Fu = g. \tag{3}$$

$$F = L + R + N. \tag{4}$$

By substituting Eqs. (4) into (3) one gets:

$$Lu + Ru + Nu = g, \tag{5}$$

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 Eq. (5) as

$$Lu = g - Ru - Nu. \tag{6}$$

By multiplying Eq. (6) by L^{-1} we obtain:

$$L^{-1}(Lu) = L^{-1}g - L^{-1}(Ru) - L^{-1}(Nu), \tag{7}$$

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

Therefore, Eq. (7) becomes

$$u = u_0 - L^{-1}(Ru) - L^{-1}(Nu), \tag{8}$$

where

$$L^{-1}(Lu) = u - u(0) - tu'(0), \tag{9}$$

$$\text{and } u_0 = u(0) + tu'(0) + L^{-1}g. \tag{10}$$

Therefore, u can be presented as a series,

$$u(x) = \sum_{n=0}^{\infty} u_n. \tag{11}$$

The non-linear term $N(u)$ will be decomposed by the infinite series of Adomian Polynomials A_n [40,41],

$$Nu = \sum_{n}^{\infty} A_n, \tag{12}$$

where the Adomian's polynomials are given by

$$A_n = \frac{1}{n!}\frac{d^n}{d\lambda^n}\left[N\left(\sum_{i=0}^{\infty}\lambda^i u_i\right)\right]\bigg|_{\lambda=0}, n = 0, 1, 2, \ldots \tag{13}$$

Concerning the convergence of the Adomian decomposition method, it was intensively studied by Cherruault [42], Cherruault and Saccomandi [43] and Abbaoui and Cherruault [44].

1.2. The variational iteration method

The variational iteration method was first proposed by He [45,46]. This method is now widely used in many fields such as Physics [47], Chemistry [48], Biomedical [49] and Engineering sciences to study linear and non-linear partial differential equations [50,51].

We can write the general form of a differential Eq. (3) as follows [52]

$$F = L + N \tag{14}$$

By substituting Eqs. (3) into (14) one gets

$$Lu + Nu = g, \tag{15}$$

where L is a linear operator, N a nonlinear operator and g is an inhomogeneous term.

He [53,54] introduced the VIM where a correction functional for Eq. (15) can be written as

$$u_{n+1}(t) = u_n(t) + \int_0^t \lambda(u_n(\xi) + N\tilde{u}_n(\xi) - g(\xi))d\xi. \tag{16}$$

In the above equation λ is a general Lagrangian multiplier, which can be identified optimally via the variational theory, and $\tilde{u}_n$ is a restricted variation which means $\delta\tilde{u}_n = 0$ [55–57]. Consequently, the solution is given by $u = \lim_{n\to\infty} u_n$.