Applications of He's methods to the steady-state population balance equation in continuous flow systems

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Abstract: The population balance equation has numerous applications in physical and engineering sciences, where one of the phases is discrete in nature. Such applications include crystallization, bubble column reactors, bioreactors, microbial cell populations, aerosols, powders, polymers and more. This contribution presents a comprehensive investigation of the semi-analytical solutions of the population balance equation (PBE) for continuous flow particulate processes. The general PBE was analytically solved using homotopy perturbation method (HPM) and variational iteration method (VIM) for particulate processes where breakage, growth, aggregation, and simultaneous breakage and aggregation take place. These semi-analytical methods overcome the crucial difficulties of numerical discretization and stability that often characterize previous solutions of the PBEs. It was found that the series solutions converged exactly to available analytical steady-state solutions of the PBE using these two methods.

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1. Introduction

The population balance equation (PBE) is used to model the particulate processes in various engineering fields such as crystallization (Ma et al. 2007; Gunawan et al. 2004), granulation (Ning 1997; Hagopood et al. 2009; Eggersdorfer and Pratsinis 2014; Chaudhury et al. 2013), polymerization (Yao et al. 2014; Ziff and McGrady 1985; Blat and Tobolsky 1945), chemical engineering (Hulburt and Katz 1964; Randolph and Larson 1988), aerosol (Jacobson 2002), and biological (Srienc 1999). These processes are characterized by the presence of a continuous phase and a dispersed phase composed of particles with a distribution of properties. This makes studying (PBE) systems an active area of research.

In Ramkrishna 1985; Kostoglou and Karabelas 1994; Kumar and Ramkrisha 1996a,b; Kumar and Ramkrisha 1997; Attarakih 2013 and Santos et al. 2013 a series of papers on the available numerical methods were discussed up to the mid-eighties to find efficient and stable numerical methods for solving the population balance equation, such as the fixed- and moving pivot methods, Dual Quadrature Method of Generalized Moments (DuQMoGeM), and Cumulative Quadrature Method of Moments (CQMOM). In recent years, some powerful and simple methods have been proposed and applied successfully in mathematical, physical and engineering problems to approximate various types of partial differential equations or integral equations, for example, the Adomian decomposition method (Adomian 1994; Adomian and Rach 1986; Wazwaz 2009), the homotopy perturbation method (He 1999a, 2000, 2004, 2005a,b) and the variational iteration method (He 1997, 1998a-b, 1999b, 2006). Furthermore, until now there are no semi-analytical techniques for steady state population balance equations have been presented in the literature. The main advantage of the techniques are the most transparent methods of solution of (PBEs) because they provide immediate and visible symbolic terms of both analytical and numerical solutions to linear as well as nonlinear integro-differential equations without linearization or discretization. The variational iteration method is now widely used by many researchers to study linear and nonlinear problems and it is based on Lagrange multiplier. The homotopy perturbation method has been used by many authors to handle a wide variety of scientific and engineering applications to solve various functional equations and it has the merits of simplicity and easy execution. In these methods, the solution is considered as the sum of an infinite series, which converges rapidly to accurate solutions. In spite of its rapid successive approximations of the exact solution, the Adomian decomposition method suffers from the complicated computational work needed for the derivation of Adomian polynomials for nonlinear terms. The steady state population balance equation (PBE) for a continuous well-mixed particulate system represents the net rate of number of particles that are

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Nomenclature

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<tr>
<th>Symbol</th>
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<tr>
<td>(a)</td>
<td>mean residence time, [s]</td>
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<tr>
<td>(n_v)</td>
<td>solution components, ([L^4])</td>
</tr>
<tr>
<td>(n(v)dv)</td>
<td>number of particles of size range (v) to (v+dv), ([L^3])</td>
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<td>(v, u)</td>
<td>particle volume, ([L^3])</td>
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Abbreviations

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<tr>
<th>Acronym</th>
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<tr>
<td>CQ MOM</td>
<td>cumulative quadrature method of moments</td>
</tr>
<tr>
<td>DuQMoGeM</td>
<td>dual quadrature method of generalized moments</td>
</tr>
<tr>
<td>HPM</td>
<td>homotopy perturbation method</td>
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<tr>
<td>PBE</td>
<td>population balance equation</td>
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<td>VIM</td>
<td>variational iteration method</td>
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formed by breakage, aggregation, growth and could be written as a follows (Randolph and Larson 1988):

\[
\frac{\partial(n(v) - n^{\text{feed}}(v))}{\partial t} + \int_{v}^{\infty} \phi(v) dv = \phi(v) \tag{1}
\]

Where \(n(v)\) is the density distribution of product stream and \(n^{\text{feed}}(v)\) the density distribution of feed stream, the second term is the convective flux along the particle internal coordinate with a growth velocity \(G(v)\).

The term on the right hand side is the net rate of particle generation by aggregation and breakage which is given by (Hulbert and Katz 1964; Prasher 1987):

\[
\phi(v) = \left\{ \begin{array}{ll}
\Gamma(v) n(v) - \int_{v}^{\infty} \alpha(v,u)n(v)n(u)du \\
\Gamma(v) n(v) + \int_{v}^{\infty} \beta(v/u) \Gamma(u) n(u)du \\
\frac{1}{2} \int_{v}^{\infty} \alpha(v-u,u)n(v)n(v-u)du
\end{array} \right. \tag{2}
\]

where \(\Gamma(v)\) and \(\alpha(v,u)\) are the breakage and aggregation frequencies, respectively, and \(\beta(v/u) dv\) is the breakage function for the formation of particles in the size range \(v+dv\) from a particle of size \(u\). The first two terms on the right hand side represent particle loss due to breakup and aggregation followed by two terms which represent particle formation due to breakup and aggregation.

Recently, these semi analytical techniques have been applied for solving (PBEs) for batch and continuous flow particulate dynamic processes (Hasseine et al. 2011; 2015a,b; Hasseine and Bart 2015). The objective of this paper is to solve certain forms of the above equation and extend the VIM and HPM techniques to derive the exact solutions of the steady state PBEs incorporating breakage, aggregation, growth, and simultaneous breakage and aggregation.

The rest of this paper is organized as follows. In Sections 2 and 3, we give an analysis of the variational iteration and homotopy perturbation methods. The analytical and numerical results for the steady state equations using the variational iteration and homotopy perturbation methods are presented in Section 4. Finally, we give our conclusions in Section 5.

2. The variational iteration method

To introduce the basic ideas of the variational iteration method (VIM), we consider the following differential equation:

\[
Lu + Nu = g(t) \tag{3}
\]

Where \(L\) is a linear operator, \(N\) a nonlinear operator and \(g(t)\) a source term. According to the VIM, we can write down a correction functional as follows:

\[
U_{n+1}(t) = U_n(t) + \int_{0}^{t} \lambda(Lu_n(\xi) + N \tilde{U}_n(\xi) - g(\xi)) d\xi \tag{4}
\]

Where \(\lambda\) is a general Lagrangian multiplier which can be identified optimally via the variational theory and \(\tilde{U}_n\) is a restricted variation which means \(\delta \tilde{U}_n = 0\) (He. 1998a,b).

Consequently, the solution is given by \(u = \lim_{n \to \infty} U_n\).

In the case of the steady state integral equations as given by Eq.(1), and since the Lagrange multiplier \(\lambda\) plays an essential role in applying the VIM method, we should differentiate both sides of this equation to obtain an equivalent integro-differential equation and consequently applying this method in a similar manner as discussed above.

3. He’s Homotopy perturbation method

To explain this method, let us consider the following function:

\[
A(u) + f(r) = 0, r \in \Omega \tag{5}
\]

with boundary conditions

\[
B(u, \frac{\partial u}{\partial n}) = 0, r \in \partial \Omega \tag{6}
\]

where \(A\) is a general differential operator, \(B\) a boundary operator, \(f(r)\) is a known analytical function and \(\partial \Omega\) is the boundary of the domain \(\Omega\). Eq. (5) can be rewritten as

\[
L(u) + N(u) - f(r) = 0 \tag{7}
\]

According to the HPM, we construct a homotopy as follows

\[
J(L(u) - f, \varepsilon) = \varepsilon J(L(u), \varepsilon) - J(f, \varepsilon) = 0
\]

where \(\varepsilon\) is a homogenization parameter to be determined.
\[ H(v,p) = L(v) - L(u_0) + pL(u_0) + p(N(v) - f(r)) = 0 \]

or

\[ H(v,p) = (1-p)[L(v) - L(u_0)] + p[A(v) - f(r)] = 0 \]

Where \( r \in \Omega \) and \( p \in [0,1] \) is an embedding parameter, \( u_0 \) is an initial approximation which satisfies the boundary conditions. Obviously, from Eq. (8), we have

\[ H(v,0) = L(v) = L(u_0) = 0 \]

(9)

\[ H(v,1) = A(v) - f(r) = 0 \]

(10)

The changing process of \( p \) from zero to unity is just that of \( v(r,p) \) from \( u_0 \) to \( u(r) \). In topology, this called deformation, \( L(v) - L(u_0) \) and \( L(v) - N(v) - f(r) \) are homotopic. The basic assumption is that the solution of Eq. (8) can be expressed as a power series in \( p \):

\[ v = v_0 + pv_1 + p^2v_2 + \cdots \]

(11)

The approximate solution of Eq. (5), therefore, can be readily obtained:

\[ u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + \cdots \]

(12)

4. Illustrative Examples

In all the following case studies, we will apply the variational iteration method and the homotopy perturbation method to solve the steady state population balance equation, and present the analytical and numerical results to verify the effectiveness of both methods.

4.1. Aggregation only with \( \omega = \omega_0 = 1 \)

Consider the steady state problem in the continuous system as given by Eq. (1) with \( \omega = \omega_0 = 1 \):

\[ \frac{[n(v) - n^{\text{ref}}(v)]}{a} = \frac{1}{2} \int_0^v n(v-u)n(v)du - \int_0^v n(u)n(v)du \]

(13)

4.1.1. Homotopy perturbation method

To solve the Eq. (13) by the HPM, we can construct the following homotopy:

\[ hp = (1-p)[n(v) - n_0(v)] + p[n(v) - n^{\text{ref}}(v)] \]

\[ -\frac{a}{2} \int_0^v n(v-u)n(u)du + \int_0^v n(u)n(v)du ] \]

(14)

with the initial distribution is assumed as follows:

\[ n_0 = n^{\text{ref}}(v) = e^{-v} \]

(15a)

Substituting Eq. (11) into Eq. (14) and equating the coefficients of \( p \) with the same power, one gets

\[ n_1(v) = \frac{a}{2} \int_0^v n(u)n_0(-u+v)du - \int_0^v n(u)n_0(v)du \]

(15b)

\[ n_2(v) = \frac{a}{2} \int_0^v n_0(-u+v)n_0(u)du + \frac{a}{2} \int_0^v n_0(u)n_0(-u+v)du - \int_0^v n_0(v)n_0(u)du \]

(15c)

\[ n_3(v) = \frac{a}{2} \int_0^v n_1(u)n_0(-u+v)du + \frac{a}{2} \int_0^v n_1(u)n_0(-u+v)du - \int_0^v n_1(v)n_0(u)du \]

(15d)

The corresponding solutions for the above system of equations are the series solution which is given as:

\[ n_1(v) = -ae^v + \frac{1}{2}ae^{-v} \]

(16a)

\[ n_2(v) = 3 \frac{a^2}{2}e^{v} - \frac{3}{2}a^2e^{v} + 1 \frac{a}{4}ae^{-v} \]

(16b)

\[ n_3(v) = -\frac{5}{2}a^3e^{v} + 15 \frac{a}{4}a^3e^{v} - \frac{5}{4}a^3e^{v} + 1 \frac{5}{48}a^3e^{-v} \]

(16c)

4.1.2. Variational iteration method

We apply variational iteration method to Eq. (13) where its iteration formula reads

\[ n_{n+1}(\xi) = n_n(\xi) - \frac{\partial}{\partial \xi} \int_0^\xi \left( \frac{n_n(u) - n^{\text{ref}}(u)}{a} \right) du \]

(17)

Substituting Eq. (15a) into Eq. (17), we have the following results

\[ n_1(v) = e^v - ae^v + \frac{1}{2}ae^{-v} \]

(18a)

\[ n_2(v) = \left( \frac{1}{2}ae^{-v} + \frac{3}{2}a^2e^{v} + 1 \frac{1}{4}ae^{-v} \right) v \]

(18b)

\[ n_3(v) = \left( e^v - ae^v - \frac{3}{2}a^2e^{v} - \frac{5}{2}a^2e^{v} + 1 \frac{15}{8}a^3e^{-v} \right) v \]

(18c)

Here the coefficient of \( a^n \) is obtained.
The general term for the two methods is:

\[
    n_n(v) = 2^{-1-n} \frac{e^{-v} \left( \frac{av}{1 + 2a} \right)^{1-n}}{\sqrt{1 + 2a} \Gamma[m] \Gamma[1 + m]} \tag{19}
\]

According to \( u = \lim_{m \to +\infty} n_n = n_0 + n_1 + n_2 + \cdots \), the exact solution is given by:

\[
    e^{v(1+u)/a} \left( \frac{1}{1 + 2a} \right)^{1-u} = \frac{1}{\sqrt{1 + 2a}} \Gamma[m] \Gamma[1 + m]
\]

\[
    n(v) = \left( \frac{1}{1 + 2a} \right)^{1-v} \frac{e^{-v}}{\sqrt{1 + 2a}} \tag{20}
\]

where \( l_0(v) \) and \( l_1(v) \) are modified Bessel Functions of the first kind of zero and first orders.

The above analytical solution is the same as that derived by (Hounslow 1990) using the Laplace transform methods.

In Fig. 1, the analytical solutions for the number density function \( n(v) \) predicted at steady state from Eq. (20) and using both VIM and HPM are compared for three different values of residence time (i.e., \( a=10, 10^3 \) and \( 10^5 \)). It is clear that the analytical results are in excellent agreement with each other. A similar behavior has been observed by (Hounslow 1990) for the case of pure aggregation from a feed exponential density function.

### 4.2. Breakage with \( \Gamma(v)=v \) and \( \beta(v/u)=2/u \)

In this section we consider the steady state problem in the continuous system with linear breakage frequency \( \Gamma(v)=v \) and a uniform daughter particle distribution \( \beta(v/u)=2/u \) where Eq.(1) is reduced to:

\[
    \frac{n(v) - n_{\text{in}}(v)}{a} = -v n(v) + 2 \int n(u) du \tag{21}
\]

as in the aggregation problem, the exponential initial distribution was used.

#### 4.2.1. Homotopy perturbation method

In order to solve the Eq. (28) by HPM, we can construct the following homotopy:

\[
h_p = (1 - p)(n(v) - n_{\text{in}}(v)) + p \left( n(v) - n_{\text{in}}(v) \right)
\]

Substituting Eq. (11), into Eq. (22) and rearranging based on powers of \( p \)-terms, one gets:

\[
    n_{\text{in}}(v) = -av n_{\text{in}}(v) + 2a \int n_{\text{in}}(v) du \tag{23a}
\]

\[
    n_{\text{in}}(v) = -av n_{\text{in}}(v) + 2a \int n_{\text{in}}(v) du \tag{23b}
\]

\[
    n_{\text{in}}(v) = -av n_{\text{in}}(v) + 2a \int n_{\text{in}}(v) du \tag{23c}
\]

The corresponding solutions for the above system of equations are the series solution which is given as:

\[
    n_{\text{in}}(v) = 2ae^{-v} - ae^{-v} \tag{24a}
\]

\[
    n_{\text{in}}(v) = 2ae^{-v} - 4ae^{-v} + a^2 e^{-v} \tag{24b}
\]

\[
    n_{\text{in}}(v) = -6a^2 e^{-v} + 6a^2 e^{-v} - a^2 e^{-v} \tag{24c}
\]

#### 4.2.2. Variational iteration method

We apply variational iteration method to Eq. (28) where its iteration formula reads:

\[
n_{\text{in}}(v) = n_{\text{in}}(v) - \frac{d}{dv} \left[ \int \left( n_{\text{in}}(\xi) - n_{\text{in}}(v) \right) d\xi \right] \tag{25}
\]

substituting Eq. (15a) into Eq. (25), we have the following results:

\[
    n_{\text{in}}(v) = e^{-v} + 2ae^{-v} - ae^{-v} \tag{26a}
\]

\[
    n_{\text{in}}(v) = e^{-v} + 2ae^{-v} + 2a^2 e^{-v} - ae^{-v} - 4a^2 e^{-v} + a^2 e^{-v} \tag{26b}
\]

\[
    n_{\text{in}}(v) = e^{-v} + 2ae^{-v} + 2a^2 e^{-v} - ae^{-v} - 4a^2 e^{-v} + 6a^2 e^{-v} - a^2 e^{-v} \tag{26c}
\]

Finally, we calculate the general term from the series solution given by the two methods (A) and (B) as follows:

\[
n_{\text{in}}(v) = \frac{e^{-v}(2 - 3m^2 + 2m^2 + 2m + 2m^2 + v^2)}{av} \tag{27}
\]

so

\[
n(v) = e^{-v} \left( \frac{1 + 2a(1 + v) + a^2(2 + 2 + v^2)}{(1 + av)^2} \tag{28}
\]

The above analytical solution is the same as that given by (Nicmanis and Hounslow 1998; Attarakih et al. 2004).

In Figure 2, the steady-state distributions calculated by the VIM and HPM are compared with the corresponding analytical given by (Nicmanis and Hounslow1998; Attarakih et al. 2004) for different values of the mean residence time (i.e. \( a=10, 10^3 \) and \( 10^5 \)). It is obvious that there is an excellent agreement between the three analytical solutions.
Fig. 2. Comparison between the VIM and HPM and the analytical solution
(Nicmanis and Houlsnou 1998; Attarakh et al. 2004) for particle breakage in
a homogeneous flow vessel with uniform daughter particle distribution
and linear breakage rate. The analytical solution is exactly identical to
those obtained by VIM and HPM.

4.3. Growth only with G=1

We consider the initial value problem in the continuous flow
system as with only particle growth involving constant growth
rate G=1 which can be obtained from Eq.(1):

\[
\frac{d}{dv}N(v) - \frac{n^\text{ind}(v)}{a} + \frac{[G N(v)]}{a} = 0
\]  

(29)

4.3.1. Homotopy perturbation method

In order to solve the Eq. (42) by the HPM, we can construct the
following homotopy:

\[
h_p = (1 - p)(n(v) - n_0(v)) + p\left(\frac{n(v) - n^\text{ind}(v)}{a} + \frac{[G N(v)]}{a}\right)
\]

(30)

With initial distribution

\[n_0(v) = -e^{-v} / a\]  

(31a)

Substituting Eq. (11) in Eq. (30) and equating the coefficients of
like powers of p, gives the following set of equations:

\[
n_1(v) = \int_0^1 \frac{n_0(v)dv}{a} = \frac{1}{a} - e^{-v}/a^2
\]

(31b)

\[
n_2(v) = \int_0^1 \frac{n_0(v)dv}{a} = \frac{1}{a} + e^{-v}/a^2 + \frac{v^2}{2a^4}
\]

(31c)

\[
n_3(v) = \int_0^1 \frac{n_0(v)dv}{a} = \frac{1}{a} + e^{-v}/a^2 + \frac{v^2}{2a^4}
\]

(31d)

4.3.2. Variational iteration method

Now we apply the variational iteration method to Eq. (42) with
the following iteration formula:

\[
n_{n+1}(v) = n_n(v) - \int_0^1 \left(\frac{n(z) - n^\text{ind}(z)}{a} + \frac{[G N(z)]}{a}\right)dz
\]

(32)

By substituting Eq. (31a) into Eq. (32), one gets the following
results:

\[
n_1(v) = e^{-v}\left(-\frac{1}{a^2} + \frac{1}{a^3}\right)
\]

(33a)

\[
n_2(v) = e^{-v}\left(-\frac{1}{a^2} + \frac{1}{a^3} - \frac{1}{a^4}\right)
\]

(33b)

\[
n_3(v) = e^{-v}\left(-\frac{1}{a^2} + \frac{1}{a^3} - \frac{1}{a^4} + \frac{1}{a^5}\right)
\]

(33c)

Accordingly, the general series term of the two methods (A) and
(B) is given as follows:

\[
n_n(v) = \frac{a(-v/a)^n}{(-1 + a)vPochhammer[1, -1 + m]} - e^{-v}\left(\frac{1}{a}\right)^{n+1}
\]

(34)

Then the closed form of the solution can be written as

\[
n(v) = \sum_{n=0}^{\infty} \frac{a(-v/a)^n}{(-1 + a)vPochhammer[1, -1 + m]} - e^{-v}\left(\frac{1}{a}\right)^{n+1}
\]

(35)

with the exact solution as:

\[
n(v) = e^{-v}\left(-1 + e^{\frac{v}{a}}\right)/(1 - a)
\]

(36)

In Figure 3, a comparison is made between the exact solutions of
Eq. (29) obtained by both VIM and HPM for the case of
constant growth rate (G = 1) for different values of the mean
residence time (i.e.,a=10, 10^3 and 10^5). The solutions are in good
agreement with each other.

4.4. Simultaneous breakage and aggregation

In this case, the analytical solution for steady state continuous
flow system is not available in the open published literature. This
case represents a combination of linear breakage rate \[\Gamma(v)=v\]
and a uniform binary daughter particle distribution \[\beta(v/a)=2/u\]
and exponential feed distribution. Using these functions Eq.(1) can be simplified into the
following continuous PBE:

\[
\frac{d}{dv}\left([N^\text{-ind}(v)]\right) + \frac{[G N(v)]}{a} = 0
\]  

(37)

\[
\frac{d}{dv}\left([N^\text{-ind}(v)]\right) + \frac{[G N(v)]}{a} = 0
\]  

(38)

\[
\frac{d}{dv}\left([N^\text{-ind}(v)]\right) + \frac{[G N(v)]}{a} = 0
\]  

(39)

\[
\frac{d}{dv}\left([N^\text{-ind}(v)]\right) + \frac{[G N(v)]}{a} = 0
\]  

(40)

Fig. 3. Comparison between the VIM and HPM for particle growth in a
homogeneous flow vessel.
The solution of the above equations yields:

\[
\begin{align*}
\xi(v) &= e^{-v}, \\
\eta(v) &= e^{-v}, \\
\delta(v) &= e^{-v}, \\
\zeta(v) &= e^{-v}.
\end{align*}
\]

Now by assuming that the solution of Eq. (56) is in the form:

\[
m(v) = \frac{p_1(v) + p_2(v) + p_3(v) + p_4(v)}{1 + w(v)},
\]

and substituting (57) into (56) and collecting terms of the same power of \( p \) one finds:

\[
m(v) = \frac{p_1(v) + p_2(v) + p_3(v) + p_4(v)}{1 + w(v)}.
\]

The application of the homotopy perturbation method to Eq. (37) results in the following formula:

\[
m(v) = \frac{1 - \eta}{\eta(w(v) - p(v))}.
\]

Fig. 4. The approximate solution for simultaneous aggregation and breakage in continuous flow systems with exponential feed distribution.
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