Solution of Population Balance Equation Using Homotopy Analysis Method

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Abstract In this paper, homotopy analysis method (HAM) is used to obtain the analytic solution for fragmentation population balance equation. Different sample problems are solved using HAM and their series solution is obtained. A detailed analysis of the series solution and the region of convergence of the solution is also studied. It is observed that the convergence region of the series solution can be adjusted with the help of certain parameters involved in HAM.

Keywords Homotopy analysis method · Population balance equation · Analytic approximations · Fragmentation · Convergence

1 Introduction

The events where two or more particles collide among each other and undergo certain changes in their physical properties are known as particulate processes. These changes can be in their mass, volume, size, entropy or some other properties of particles. Population balance equations (or PBEs) are basically integro-partial differential equations which represent the change in the particle properties present in a system due to particulate process. Various examples of these events can be seen in different fields of science and engineering like the formation of stars, growth of gas bubbles in solids, merging of drops in atmospheric clouds, and so on [1].

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In this paper, the PBE considered represents particle fragmentation. Fragmentation is a process where a particle break into two or more smaller (or daughter) fragments. The total number of particles present in the closed system increases due to fragmentation. Let $c(t, x)$ denote the number density of particles of volume $x \geq 0$ at time $t \geq 0$ in a system undergoing particulate process (fragmentation). In this regard, for $(t, x) \in [0, T] \times [0, \infty)$ where $T < \infty$, the general fragmentation population balance equation is written as [2]

$$\frac{\partial c(t,x)}{\partial t} = 2\int_{x}^{\infty} F(x, y-x)c(t,y)\mathrm{d}y - c(t,x)\int_{0}^{x} F(x-y, y)\mathrm{d}y, \tag{1}$$

with the initial data

$$c(0, x) = c_0(x) \geq 0, \quad \text{for all} \quad x \geq 0. \tag{2}$$

The left hand side (lhs) of equation (1) gives the time evolution of particle number density $c(t, x)$. In the right hand side (rhs), the function $F(x, y)$ represents the rate at which the particles of size $x + y$ breaks into particles of size x and size y. The first term indicates the inclusion (or birth) of $x-$size particles in the system, and the second term indicates the removal (death) of $x-$size particles from the system.

Several numerical, semi-analytical, and analytical methods have been devised over the years to solve PBE. For fragmentation problems, one can refer to the articles [2, 3] for exact solutions and the articles [4, 5] for numerical solutions. To our knowledge, the homotopy analysis method (HAM) has not been used to solve the fragmentation problem to date, and this is the first attempt to solve above mentioned PBE with HAM.

HAM was first introduced by Liao [6] in 1992 to solve different linear and non-linear differential equations appearing in the physical systems. Over the years, HAM has received sincere attention from the researchers due to its ability to solve different complicated real-life problems. This is an analytic method which uses the concept of homotopy from topology to generate a convergent series solution to the considered problem. In HAM, we construct deformation equations with the help of initial guess of the solution, auxiliary linear operator, auxiliary parameter, and auxiliary function, and we have great freedom to choose all of these. Because of this freedom, this method is very flexible and convenient to use as compared to other methods like Adomian decommission method, artificial parameter method, perturbation method, etc.

The outline of this paper is as follows. In Sect. 2, the preliminary idea of homotopy analysis method is discussed. In Sect. 3, HAM is applied to solve the particulate problem (1)−(2) mentioned in Sect. 1 and its convergence is discussed. In Sect. 4, some sample examples are solved using the software Mathematica 12.2, and the efficiency of the method is discussed. Finally, the conclusion of the present work is discussed in Sect. 5.

2 Preliminaries: Homotopy Analysis Method

The key methodology of HAM is to approximate the solution $c(t, x)$ in terms of a series of functions. In this regard, we consider $c_0(t, x)$ as an initial guess of the solution. Let us now define an unknown function $v(t, x; q)$, where t and x are independent variables and $q \in [0, 1]$ is the embedding parameter. The underlying idea of HAM is that a continuous mapping is described to relate the solution $c(t, x)$ and the unknown function v, with the aid of the embedding-parameter q. Thus, the initial guess $c_0(t, x)$ of the solution $c(t, x)$ is so chosen that $v(t, x; q)$ varies from $c_0(t, x)$ to $c(t, x)$ as q varies from 0 to 1. Representing this mathematically, we can write $v(t, x; 0) = c_0(t, x)$ and $v(t, x; 1) = c(t, x)$. To ensure the above relation, a linear operator $\mathscr{L}[v(t, x; q)]$, an auxiliary parameter $\hbar$ ($\neq 0$) and an auxiliary function $H(t, x)$ are needed to be defined wisely. Under all these considerations, let us discuss the homotopy analysis method.

Let the initial assumption to the solution is independent of t and coincides with the initial data (2), that is

$$c_0(t, x) = c(0, x). \tag{3}$$

Choose the linear operator with

$$\mathscr{L}[v(t, x; q)] = \frac{\partial v(t, x; q)}{\partial t} \tag{4}$$

such that

$$\mathscr{L}[f(x, y)] = 0 \iff f(x, y) = 0. \tag{5}$$

Let us consider the generalized problem in the following operator form

$$\mathscr{N}[c(t, x)] = 0. \tag{6}$$

Using embedding parameter, we can construct a homotopy

$$\begin{aligned}\mathscr{H}[v(t, x; q); q, \hbar, H] := (1 - q)\mathscr{L}[v(t, x; q) - c_0(t, x)]\\ - q\hbar H(t, x)\mathscr{N}[v(t, x; q)] = 0.\end{aligned} \tag{7}$$

For $q = 0$, Eq. (7) along with (5) gives

$$\mathscr{L}[v(t, x; 0) - c_0(t, x)] = 0 \quad \text{imples} \quad v(t, x; 0) = c_0(t, x). \tag{8}$$

Again for $q = 1$, since $\hbar \neq 0$ and $H(t, x) \neq 0$, relation (7) becomes

$$\mathscr{N}[v(t, x; 1)] = 0, \tag{9}$$

which replicates the original problem (6), provided

$$v(t, x; 1) = c(t, x). \tag{10}$$

According to Eqs. (8) and (10), $v(t, x; q)$ varies from the initial guess $c_0(t, x)$ to the exact solution $c(t, x)$ as the embedding parameter q varies from 0 to 1. The equation (7) is called *zero-order deformation equation*.

The freedom to choose $\mathscr{L}$, $c_0(t, x)$, $\hbar$, $H(t, x)$, enables us to adjust all the parameters properly such that the solution of deformation equation exists for $q \in [0, 1]$. The $m-$th order derivative of $c_0(t, x)$ with respect to embedding parameter q is defined as

$$c^{[m]}(t, x) := \frac{c_0^{[m]}(t, x)}{m!} = \frac{1}{m!} \frac{\partial^m v(t, x; q)}{\partial q^m}\bigg|_{q=0}. \tag{11}$$

By Taylor's theorem, $v(t, x; q)$ can be expanded in a power series of q as

$$v(t, x; q) = v(t, x; 0) + \sum_{m=1}^{\infty} \frac{c_0^{[m]}(t, x)}{m!} q^m = f(x) + \sum_{m=1}^{\infty} c^{[m]}(t, x) q^m. \tag{12}$$

In general, the above series will converge for $q = 1$, and hence using relation (9), we have

$$c(t, x) = f(x) + \sum_{m=1}^{\infty} c^{[m]}(t, x). \tag{13}$$

We define the vector $\vec{c}_n := \{c_0(t, x), c_1(t, x), c_2(t, x), \ldots, c_n(t, x)\}$. Differentiating zero-order deformation (7) $m-$times with respect to q, then dividing it by $m!$, and finally setting $q = 0$, we get the following $m-$th order deformation equation:

$$\mathscr{L}[c_m(t, x) - \chi_m c_{m-1}(t, x)] = \hbar H(t, x) R_m(\vec{c}_{m-1}, t, x) \tag{14}$$

with initial condition $c_m(0, x) = 0$, where $\chi_m := \begin{cases} 0, & \text{when } m \leq 1, \\ 1, & \text{when } m > 1. \end{cases}$ and

$$\begin{aligned} R_m(\vec{c}_{m-1}, t, x) &= \frac{1}{(m-1)!} \frac{\partial^{m-1} \mathscr{N}[v(t, x; q)]}{\partial q^{m-1}}\bigg|_{q=0} \\ &= \frac{1}{(m-1)!} \frac{\partial^{m-1}}{\partial q^{m-1}} \mathscr{N}\left[\sum_{n=0}^{\infty} c_n(t, x) q^n\right]_{q=0}. \end{aligned} \tag{15}$$

Thus, the solution to problem is reduced to

$$c_m(t,x) = \chi_m c_{m-1}(t,x)] + \int_0^t \hbar H(t,s) R_m(\vec{c}_{m-1}, s, x). \tag{16}$$

where R_m is given by (15).

3 HAM Based Solutions and Convergence Theorem

For (1)−(2) the operator $\mathcal{N}$ is given by

$$\mathcal{N}[v(t,x;q)] = \frac{\partial v(t,x;q)}{\partial t} - 2\int_x^\infty F(x, y-x) v(t,y;q)\mathrm{d}y - v(t,x;q)\int_0^x F(x-y, y)\mathrm{d}y.$$

Using (15), we can calculate R_m for $m = 1, 2, 3, \ldots$ as shown below

$$\begin{aligned} R_1(\vec{c}_0, t, x) &= \mathcal{N}[c_0(t,x)]|_{q=0} \\ &= -2\int_x^\infty F(x, y-x) c_0(t,y)\mathrm{d}y \\ &\quad - c_0(t,x)\int_0^x F(x-y, y)\mathrm{d}y. \end{aligned} \tag{17}$$

For $m = 2$,

$$\begin{aligned} R_2(\vec{c}_1, t, x) &= \left[\frac{\partial}{\partial q}\mathcal{N}\left[c_0(t,x) + c_1(t,x)q\right]\right]_{q=0} \\ &= \frac{\partial c_1(t,x)}{\partial t} - 2\int_x^\infty F(x, y-x) c_1(t,y)\mathrm{d}y \\ &\quad - c_1(t,x)\int_0^x F(x-y, y)\mathrm{d}y. \end{aligned} \tag{18}$$

For $m = 3$,

$$\begin{aligned} R_3(\vec{c}_2, t, x) &= \frac{1}{2!}\left[\frac{\partial^2}{\partial q^2}\mathcal{N}\left[c_0(t,x) + c_1(t,x)q + c_2(t,x)q^2\right]\right]_{q=0} \\ &= \frac{\partial c_2(t,x)}{\partial t} - 2\int_x^\infty F(x, y-x) c_2(t,y)\mathrm{d}y \\ &\quad - c_2(t,x)\int_0^x F(x-y, y)\mathrm{d}y. \end{aligned} \tag{19}$$

Likewise the mth order representation is

$$\begin{aligned} R_m\left(\vec{c}_{m-1}, t, x\right) = & \frac{\partial c_{m-1}(t, x)}{\partial t} \\ & - 2\int_x^{\infty} F(x, y-x) c_{m-1}(t, y) \mathrm{d}y \\ & - c_{m-1}(t, x) \int_0^x F(x-y, y) \mathrm{d}y. \end{aligned} \tag{20}$$

Thus, the solution to fragmentation equation (1)–(2) for $H(t, x) = 1$ is written as

$$c_m(t, x) = \chi_m c_{m-1}(t, x)] + \int_0^t h R_m\left(\vec{c}_{m-1}, s, x\right), \tag{21}$$

where R_m is given by (20).

Theorem 1 *As long as the series* (13) *converges, where* $c_m(t, x)$ *is governed by the high order deformation equation* (14) *under the conditions* (15) *and* (16)*, it must be the exact solution of* (1)–(2).

Proof If the series $\sum_{m=0}^{\infty} c_m(t, x)$ converges, then we can write

$$v(t, x) = \sum_{m=0}^{\infty} c_m(t, x), \quad \text{that is} \quad \lim_{m \to \infty} c_m(t, x) = 0. \tag{22}$$

In this context

$$\sum_{m=0}^{n} \left[c_m(t, x) - \chi_m c_{m-1}(t, x)\right] = c_1 + (c_2 - c_1) + \cdots + (c_n - c_{n-1}) = c_n(t, x),$$

and hence in accordance with relation (22), we get

$$\sum_{m=0}^{\infty} \left[c_m(t, x) - \chi_m c_{m-1}(t, x)\right] = \lim_{n \to \infty} c_n(t, x) = 0.$$

Due to the linearity property of $\mathscr{L}$, we have

$$\sum_{m=0}^{\infty} \mathscr{L}\left[c_m(t, x) - \chi_m c_{m-1}(t, x)\right] = \mathscr{L} \sum_{m=0}^{\infty} \left[c_m(t, x) - \chi_m c_{m-1}(t, x)\right] = 0.$$

Thus recalling (14), we obtain

$$\sum_{m=0}^{\infty} \mathscr{L}\left[c_m(t,x) - \chi_m c_{m-1}(t,x)\right] = \hbar H(t,x) \sum_{m=1}^{\infty} R_m\left[\vec{c}_{m-1}\right] = 0.$$

Since $\hbar \neq 0$ and $H(t,x) \neq 0$, therefore

$$\sum_{m=1}^{\infty} R_m\left[\vec{c}_{m-1}\right] = 0. \tag{23}$$

Recalling (22), we get

$$\begin{aligned}
\sum_{m=1}^{\infty} R_m\left[\vec{c}_{m-1}\right] &= \sum_{m=1}^{\infty}\left[\frac{\partial c_{m-1}(t,x)}{\partial t} \quad - 2\int_x^{\infty} F(x, y-x) c_{m-1}(t,y)\mathrm{d}y - c_{m-1}(t,x)\right. \\
&\quad \left. \int_0^x F(x-y, y)\mathrm{d}y\right] \\
&= \sum_{m=1}^{\infty} \frac{\partial c_{m-1}(t,x)}{\partial t} - 2\int_x^{\infty} F(x, y-x) \sum_{m=1}^{\infty} c_{m-1}(t,y)\mathrm{d}y \\
&\quad - \sum_{m=1}^{\infty} c_{m-1}(t,x) \int_0^x F(x-y,y)\mathrm{d}y \\
&= \frac{\partial}{\partial t} \sum_{m=1}^{\infty} c_{m-1}(t,x) - 2\int_x^{\infty} F(x, y-x) \sum_{m=1}^{\infty} c_{m-1}(t,y)\mathrm{d}y \\
&\quad - \sum_{m=1}^{\infty} c_{m-1}(t,x) \int_0^x F(x-y,y)\mathrm{d}y \\
&= \frac{\partial}{\partial t} \sum_{m=0}^{\infty} c_m(t,x) - 2\int_x^{\infty} F(x, y-x) \sum_{m=0}^{\infty} c_m(t,y)\mathrm{d}y \\
&\quad - \sum_{m=0}^{\infty} c_m(t,x) \int_0^x F(x-y,y)\mathrm{d}y.
\end{aligned}$$

Combining (22) and (23), we have

$$\frac{\partial v(t,x)}{\partial t} = 2\int_x^{\infty} F(x, y-x) v(t,y)\mathrm{d}y - v(t,x) \int_0^x F(x-y,y)\mathrm{d}y. \tag{24}$$

Now, from the initial conditions of $c_m(t,x)$, it holds that

$$v(0,x) = \sum_{m=0}^{\infty} c_m(0,x) = c_0(0,x) + \sum_{m=1}^{\infty} c_m(0,x) = c_0(0,x) = c(0,x).$$

Hence, from last two expressions, one can observe that $v(t, x)$ must be the exact solution of (1)–(2).

4 Numerical Examples and Discussions

In this section, we will consider some examples discussed in [3] and will discuss using graphs how the approximate solution is approaching the exact solution.

Example 1 Let us consider (1)–(2) with $K(x, y) = 1$ and the initial condition $c(0, x) = \exp(-x)$. The exact solution to this problem is $c(t, x) = (1+t)^2 \exp(-x(1+t))$.

Using the recursive scheme (21) along with (20), we obtain $c_m(t, x)$ for $m \geq 1$ as

$$\begin{aligned} c_1(t,x) &= ht(e^{-x}x - 2e^{-x}), \\ c_2(t,x) &= h(\frac{1}{2}t^2(hx(e^{-x}x - 2e^{-x}) - 2\,he^{-x}(x-1)) + ht(e^{-x}x - 2e^{-x})), \\ c_3(t,x) &= h(\frac{1}{6}h^2t^3e^{-x}x^3 - h^2t^3e^{-x}x^2 + h^2t^2e^{-x}x^2 + h^2t^3e^{-x}x + 2\,h^2t^2e^{-x} \\ &\quad - 4\,h^2t^2e^{-x}x - 2\,h^2te^{-x} + h^2te^{-x}x). \end{aligned}$$

We have great freedom to choose $\hbar$, so we will now look for a set of values of $\hbar$ for which the solution obtained by HAM converges to the exact solution. From Fig. 1, we can observe that when $\hbar$ is near -0.5, the graph is flat. So, method will converge to the exact solution when $\hbar$ is near -0.5. Now, we will analyze graphs for different values of $\hbar$ for which the solution obtained by HAM converges to exact solution.

During the computation of graphs for several values of $\hbar$ near -0.4 and -0.2, it was observed from Fig. 2 that for $\hbar = -0.4$ the graph of 4−th, 6−th, 8−th and 10−th

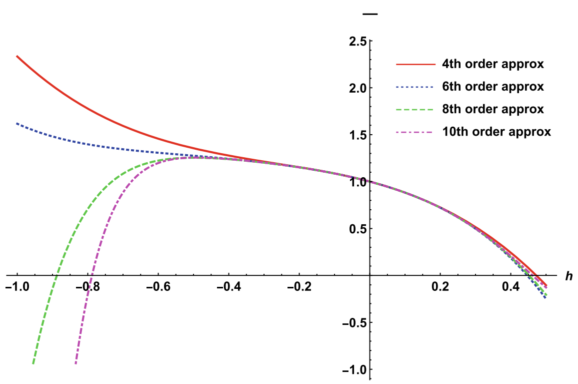
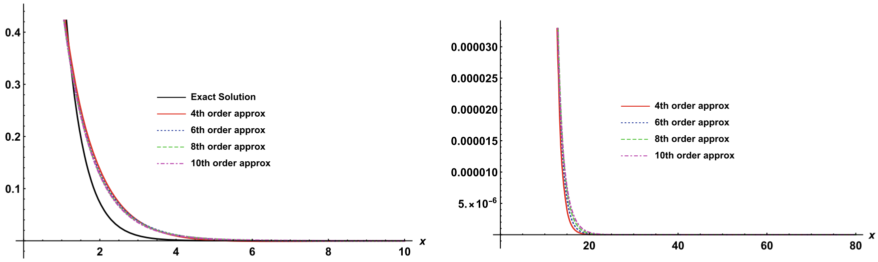


Fig. 1 $\hbar$ against $c(x, t)$ for $t = 1$ and $x = 1$ for different order of approximation for Eqs. (1)–(2)



(a) Number density

(b) Error

Fig. 2 Graph with $\hbar = -0.4$ for different order of approximation for Eqs. (1)–(2)

Table 1 Error for Example 1 when $\hbar = -0.4$

$m-$th order of approximation	4	6	8	10
Error	7.7606×10^{-5}	7.6782×10^{-5}	7.6403×10^{-5}	7.0951×10^{-5}

order approximation nearly coincides with the exact solution. Here we compute the numerical number density with the particle size distribution in Fig. 2a. On the other hand, Fig. 2b represents the numerical error curve obtained for different order approximations. For a detailed quantitative error analysis, we present the numerical errors in Table 1. To calculate the error, we recall the formula given in [5]. The following results supports that HAM predicts the solution with high accuracy even for a small number of approximate terms.

Example 2 Next consider (1)–(2) with $K(x, y) = x + y$ and the initial condition $c(0, x) = \exp(-x)$. The exact solution to this problem is $c(t, x) = \exp(-tx^2 - x)(1 + 2t(1 + x))$.

Again using the recursive scheme (21) along with (20), we obtain $c_m(t, x)$ for $m \geq 1$ as

$$
\begin{aligned}
c_1(t,x) &= ht(e^{-x}x^2 - 2e^{-x}(x+1)),\\
c_2(t,x) &= h(\frac{1}{2}t^2(hx^2(e^{-x}x^2 - 2e^{-x}(x+1)) - 2\,he^{-x}x^2(x+1)) + ht(e^{-x}x^2 \\
&\quad - 2e^{-x}(x+1))),\\
c_3(t,x) &= h(\frac{1}{6}h^2t^3e^{-x}x^6 - h^2t^3e^{-x}x^5 - h^2t^3e^{-x}x^4 + h^2t^2e^{-x}x^4 \\
&\quad - 4\,h^2t^2e^{-x}x^3 - 4\,h^2t^2e^{-x}x^2 + h^2te^{-x}x^2 - 2\,h^2te^{-x}x - 2\,h^2te^{-x}).
\end{aligned}
$$

Similar to the previous example, we will make use of graphs to investigate the value of $\hbar$ for which the series solution obtained by HAM method converges to exact solution. From Fig. 3, it is observed that graph is flat in between -0.4 and 0.

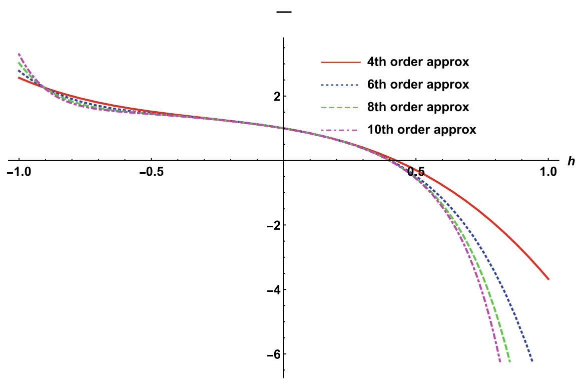


Fig. 3 $\hbar$ against $c(x, t)$ for $t = 1$ and $x = 1$ for different order of approximation for Eqs. (1)–(2)

Table 2 Error for Example 2 when $\hbar = -0.125$

$m-$th order of approximation	4	6	8	10
Error	2.9075×10^{-5}	2.8762×10^{-5}	2.8501×10^{-5}	2.8417×10^{-5}

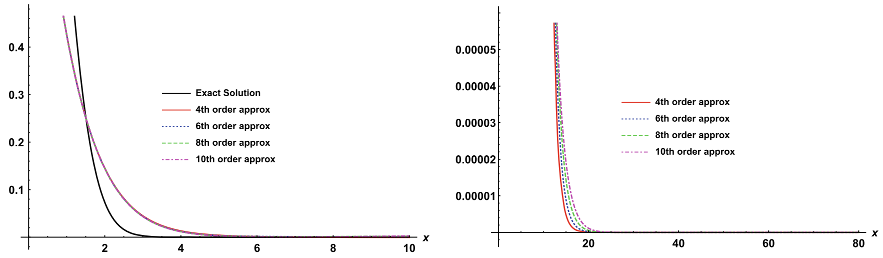


Fig. 4 Graph with $\hbar = -0.125$ for different order of approximation for Eqs. (1)–(2)

Therefore, the approximate solution will converge to exact solution somewhere in between these two points.

For a detailed investigation, we will plot the solution with respect to x for different values of $\hbar$ and it is observed that for $h = -0.125$ graph coincides with the exact solution. For a qualitative analysis of the method, we will plot the numerical solution as well as the error graph. For quantitative analysis, we present the error Table 2. Like before, it is observed that the HAM produces very accurate results for a very small number of terms and $\hbar = -0.125$ (Fig. 3).

5 Conclusion

The homotopy analysis method is applied to fragmentation PBE. A recursive scheme in the form of series solution is obtained to estimate the solution of PBEs. The convergence analysis shows that approximate solution will converge to exact solution. Error estimate for the sample problems is minimal which guarantees the accuracy of the method.

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