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Series solution of the Smoluchowski's coagulation equation

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KEYWORDS

The Smoluchowski coagulation equation; Homotopy perturbation method; Approximate solution; Error analysis; Maple software package **Abstract** The Smoluchowski coagulation equation is a mean-field model for the growth of clusters (particles, droplets, etc.) by binary coalescence; that is, the driving growth mechanism is the merger of two particles into a single one. In this study, we consider obtaining approximate solutions of the Smoluchowski's coagulation equation using the homotopy perturbation method. The numerical solutions are compared with the exact solutions. Results derived from our method are shown graphically.

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1. Introduction

Smoluchowski's equation is widely applied to describe the time evolution of the cluster-size distribution during aggregation processes. Analytical solutions for this equation, however, are known only for a very limited number of kernels. Therefore, numerical methods have to be used to describe the time evolution of the cluster-size distribution. A numerical technique is presented for the solution of the homogeneous Smoluchowski's coagulation equation with constant kernel.

In this paper, we will consider the following Smoluchowski's coagulation equation (Ranjbar et al., in press; Filbert and Laurençot, 2004):

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$$\partial_t f(x,t) = C^+(f) - C^-(f), \quad (x,t) \in R^2_+,$$
(1)

$$0) = f_0, \quad x \in \mathbb{R}_+, \tag{2}$$

f(x,0) where

$$C^{+}(f) = \frac{1}{2} \int_{0}^{x} K(x - y, y) f(x - y, t) f(y, t) dy,$$
(3)

$$C^{-}(f) = \int_{0}^{\infty} K(x, y) f(x, t) f(y, t) dy$$
(4)

and f_0 is a known value. f(x, t) is the density of cluster of mass x per unit volume at time t.

Clusters of masses x and y coalesce by binary collisions at a rate governed by a symmetric kernel K(x, y). The coagulation kernel K(x, y) characterizes the rate at which the coalescence of the two clusters with respective masses x and y produces a cluster of mass x + y and is a non-negative symmetric function

$$0 \leq K(x, y) = K(y, x), \quad (x, y) \in R^2_+.$$
 (5)

The integral in Eq. (3) accounts for the formation of the cluster of mass x resulting from the merger of two clusters with respective masses y and x - y, $y \in (0, \infty)$. The integral in Eq. (4) describes the loss of the cluster of mass x by coagulation with other clusters. Problems involving Smoluchowski's equation have received a considerable amount of attention in

the literature (Drake, 1972). Eq. (1) has been used in a wide range of applications, such as the formation of clouds and smog (Friedlander, 1977), the clustering of planets, stores, galaxies (Silk and White, 1978), the kinetics of polymerization (Ziff, 1980) and even the schooling of fishes (Niwa, 1998) and the formation of marine snow (Kiorbe, 2001). Also, an influential survey article by Aldous summarizes the recent state of affairs (Aldous, 1999). It is well known that during each coagulation event, the total mass of clusters is conserved while the number of clusters decreases. In terms of f, the total number of clusters N(t) and total mass of clusters M(t) at time $t \ge 0$ are obtained by

$$N(t) := \int_0^\infty f(x, t) dx,$$
(6)

$$M(t) := \int_0^\infty x f(x, t) dx.$$
⁽⁷⁾

While it is easy to check that N(t) is a non-increasing function of time, it is well known that M(t) might not remain constant throughout time evolution for some coagulation coefficient K(x,y) (Ernst et al., 1984). Recently, Filbert and Laurençot (2004) used a numerical scheme for the Smoluchowski coagulation equation, which relies on a conservative formulation and a finite volume approach. Also Ranjbar et al. (in press) used Taylor polynomials and radial basis functions together to solve the equation. In this paper, we will use the homotopy perturbation method for solving the Smoluchowski's coagulation equation.

He (1999, 2003, 2006a) proposed a perturbation technique, so called He's homotopy perturbation method (HPM), which does not require a small parameter in the equation and takes the full advantage of the traditional perturbation methods and the homotopy techniques. Relatively recent survey on the method and its applications can be found in Dehghan and Shakeri (2008a), Dehghan and Shakeri (2008b), Saadatmandi et al. (2009), Yıldırım (2008a,b, 2009a), Dehghan and Shakeri (2007), Shakeri and Dehghan (2008), Yıldırım (2009b), Koçak and Yıldırım (2009), Yıldırım (2008c, 2009c), and He (2008a,b, 2006b,c).

2. The homotopy perturbation method

Consider the following nonlinear differential equation:

$$A(u) - f(r) = 0, \quad r \in \Omega \tag{8}$$

with boundary conditions

$$B(u, \partial u/\partial n) = 0, \quad r \in \Gamma, \tag{9}$$

where A is a general differential operator, B is a boundary operator, f(r) is a known analytic function, and Γ is the boundary of the domain Ω .

The operator A can, generally speaking, be divided into two parts L and N, where L is linear and N is nonlinear, therefore Eq. (8) can be written as,

$$L(u) + N(u) - f(r) = 0.$$
 (10)

By using homotopy technique, one can construct a homotopy $v(r,p): \Omega \times [0,1] \to \Re$ which satisfies

$$H(v,p) = (1-p)[L(v) - L(u_0)] + p[A(v) - f(r)] = 0$$
(11a)
or

$$H(v,p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0, \quad (11b)$$

where $p \in [0, 1]$ is an embedding parameter and u_0 is the initial approximation of Eq. (8) which satisfies the boundary conditions. Clearly, we have

$$H(v,0) = L(v) - L(u_0) = 0$$
(12)

or

$$H(v,1) = A(v) - f(r) = 0$$
(13)

The changing process of p from zero to unity is just that of v(r,p) changing from $u_0(r)$ to u(r). This is called deformation, and also, $L(v) - L(u_0)$ and A(v) - f(r) are called homotopic in topology. If the embedding parameter p ($0 \le p \le 1$) is considered as a "small parameter", applying the classical perturbation technique, we can assume that the solution of Eq. (11) can be given as a power series in p, i.e.,

$$v = v_0 + pv_1 + p^2 v_2 + \cdots$$
 (14)

and setting p = 1 results in the approximate solution of Eq. (8) as

$$u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + \cdots$$
(15)

3. Numerical results and comparison with explicit solutions

Example 1. We first consider Eqs. (1)–(4) with constant kernel K(x, y) = 1 and $f_0 = \exp(-x)$ (Ranjbar et al., in press),

$$\partial_t f(x,t) = \frac{1}{2} \int_0^x f(x-y,t) f(y,t) dy - \int_0^\infty f(x,t) f(y,t) dy, \quad (16)$$

$$f(x,0) = \exp(-x),\tag{17}$$

which has exact solution as follows (Ranjbar et al., in press):

$$f(x, t) = N^{2}(t) \exp(-N(t)x) \text{ with } N(t)$$

= $\frac{2M_{0}}{2+M_{0}t}$ and $M_{0} = 1$ (18)

for $(x, t) \in \mathbb{R}^2_+$, where N(t) is the total number of particles defined by Eq. (6). In order to solve Eqs. (16) and (17) by the homotopy perturbation method, we construct the following homotopy

$$\frac{\partial f(x,t)}{\partial t} = p\left(\frac{1}{2}\int_0^x f(x-y,t)f(y,t)dy - \int_0^\infty f(x,t)f(y,t)dy\right).$$
(19)

Assume the solution of Eq. (16) in the form:

$$f(x,t) = p^0 f_0(x,t) + p^1 f_1(x,t) + p^2 f_2(x,t) + p^3 f_3(x,t) + \cdots$$
(20)

Substituting (20) into (19) and collecting terms of the same power of p give:

$$p^{0}: \frac{df_{0}(x,t)}{dt} = 0, \quad f_{0}(0,x) = f(x,0),$$

$$p^{1}: \frac{df_{1}(x,t)}{dt} = \frac{1}{2} \int_{0}^{x} f_{0}(x-y,t) f_{0}(y,t) dy$$

$$- \int_{0}^{\infty} f_{0}(x,t) f_{0}(y,t) dy, \quad f_{1}(x,0) = 0,$$

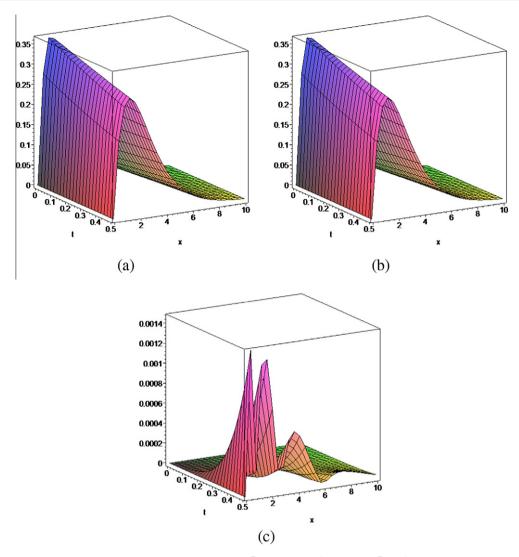


Figure 1 (a) xf(x,t), (b) $x\bar{f}(x,t)$ and (c) $|xf(x,t) - x\bar{f}(x,t)|$.

$$p^{2}: \frac{df_{2}(x,t)}{dt} = \frac{1}{2} \int_{0}^{x} (f_{0}(x-y,t)f_{1}(y,t) + f_{1}(x-y,t)f_{0}(y,t))dy \\ - \int_{0}^{\infty} (f_{0}(x,t)f_{1}(y,t) + f_{1}(x,t)f_{0}(y,t))dy, \\ f_{2}(x,0) = 0, \\ p^{3}: \frac{df_{3}(x,t)}{dt} = \frac{1}{2} \int_{0}^{x} (f_{0}(x-y,t)f_{2}(y,t) + f_{1}(x-y,t)f_{1}(y,t) \\ + f_{2}(x-y,t)f_{0}(y,t))dy - \int_{0}^{\infty} (f_{0}(x,t)f_{2}(y,t) \\ + f_{1}(x,t)f_{1}(y,t) + f_{2}(x,t)f_{0}(y,t))dy, \\ f_{3}(x,0) = 0, \end{cases}$$

solving above equations by MAPLE yields:

. . .

$$f_0(x,t) = \exp(-x),$$

$$f_1(x,t) = \frac{1}{2}(x-2)\exp(-x)t,$$

$$f_2(x,t) = \frac{1}{8}(6-6x+x^2)\exp(-x)t^2,$$

$$f_3(x,t) = \frac{1}{48}(-24+36x-12x^2+x^3)\exp(-x)t^3,$$

...

and so on, other components are easily obtained by using (19) and MAPLE. A few terms approximation to the solution of Eqs. (16) and (17) can be obtained by setting p = 1 in (20). We get the third-order approximation solution as follows:

$$\bar{f}(x,t) = \sum_{i=0}^{3} f_i(x,t) = \exp(-x)$$

$$\times \left(1 + \frac{1}{2}(x-2)t + \frac{1}{8}(6 - 6x + x^2)t^2 + \frac{1}{48}(-24 + 36x - 12x^2 + x^3)t^3\right).$$
(21)

Figs. 1 and 2 show that the numerical approximate solution has a high degree of accuracy. As we know, more the terms added to the approximate solution, more the accurate it will be. Although we only considered third-order approximation, it achieves a high level of accuracy.

Example 2. We now consider Eqs. (1)–(4) with the multiplicative coagulation kernel K(x, y) = xy and $f_0 = \exp(-x)/x$ (Ranjbar et al., in press),

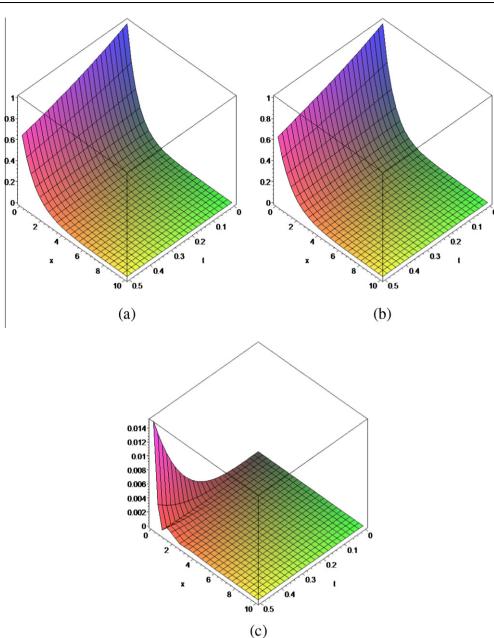


Figure 2 (a) f(x,t), (b) $\bar{f}(x,t)$ and (c) $|f(x,t) - \bar{f}(x,t)|$.

$$\partial_t f(x,t) = \frac{1}{2} \int_0^x ((x-y)y) f(x-y,t) f(y,t) dy - \int_0^\infty (xy) f(x,t) f(y,t) dy,$$
(22)

$$f(x,0) = \exp(-x)/x,$$
(23)

which has exact solution as follows (Ranjbar et al., in press):

$$f(x,t) = \exp(-Tx)\frac{I_1(2xt^{1/2})}{x^2t^{1/2}},$$
(24)

where

$$T = \begin{cases} 1+t, & t \leq 1, \\ 2t^{1/2}, & \text{otherwise} \end{cases}$$
(25)

and I_1 is the modified Bessel function of the first kind

$$I_1(x) = \frac{1}{\pi} \int_0^{\pi} \exp(x \cos \theta) \cos \theta \, d\theta.$$
 (26)

For this solution, the total volume $M_1(t)$ defined by (7) satisfies $M_1(t) = 1$ if $t \in [0, 1]$ and $M_1(t) = t^{-1/2}$ if $t \ge 1$ (and the gelation phenomenon takes place at t = 1).

Similar to previous example, we construct the following homotopy

$$\frac{\partial f(x,t)}{\partial t} = p\left(\frac{1}{2}\int_0^x ((x-y)y)f(x-y,t)f(y,t)dy - \int_0^\infty (xy)f(x,t)f(y,t)dy\right).$$
(27)

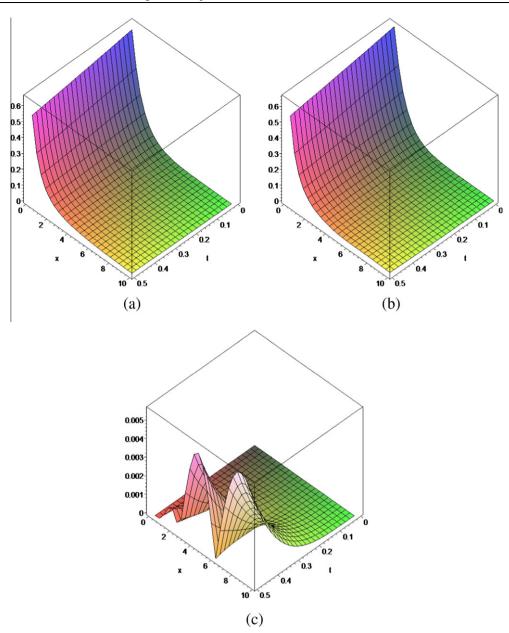


Figure 3 (a) xf(x,t), (b) $x\bar{f}(x,t)$ and (c) $|xf(x,t) - x\bar{f}(x,t)|$.

Assume the solution of Eq. (27) in the form: $f(x,t) = p^{0}f_{0}(x,t) + p^{1}f_{1}(x,t) + p^{2}f_{2}(x,t) + p^{3}f_{3}(x,t) + \cdots$ $+ \cdots$ (28)

Substituting (28) into (27) and collecting terms of the same power of p give:

$$p^{0}: \frac{df_{0}(x,t)}{dt} = 0, \quad f_{0}(0,x) = f(x,0),$$

$$p^{1}: \frac{df_{1}(x,t)}{dt} = \frac{1}{2} \int_{0}^{x} ((x-y)y)f_{0}(x-y,t)f_{0}(y,t)dy$$

$$- \int_{0}^{\infty} (xy)f_{0}(x,t)f_{0}(y,t)dy, \quad f_{1}(x,0) = 0,$$

$$p^{2}: \frac{df_{2}(x,t)}{dt} = \frac{1}{2} \int_{0}^{x} ((x-y)y)(f_{0}(x-y,t)f_{1}(y,t) + f_{1}(x-y,t)f_{0}(y,t))dy - \int_{0}^{\infty} (xy)(f_{0}(x,t)f_{1}(y,t) + f_{1}(x,t)f_{0}(y,t))dy, \quad f_{2}(x,0) = 0,$$

$$p^{3}: \frac{df_{3}(x,t)}{dt} = \frac{1}{2} \int_{0}^{x} ((x-y)y)(f_{0}(x-y,t)f_{2}(y,t) + f_{1}(x-y,t)f_{1}(y,t) + f_{2}(x-y,t)f_{0}(y,t))dy - \int_{0}^{\infty} (xy)(f_{0}(x,t)f_{2}(y,t) + f_{1}(x,t)f_{1}(y,t) + f_{2}(x,t)f_{0}(y,t))dy, \quad f_{3}(x,0) = 0, \dots$$

solving above equations by MAPLE yields:

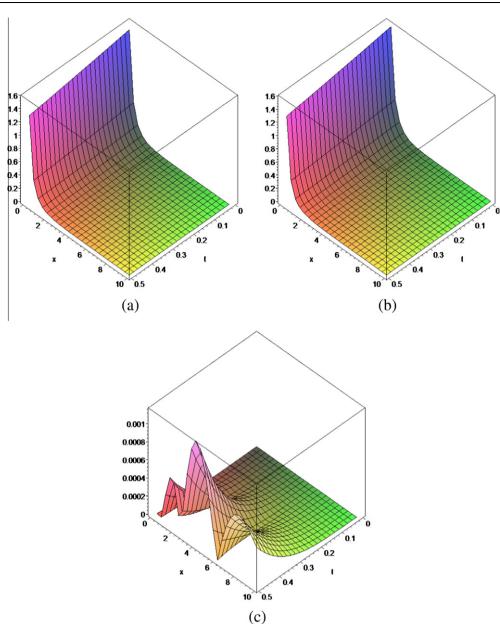


Figure 4 (a) f(x, t), (b) $\bar{f}(x, t)$ and (c) $|f(x, t) - \bar{f}(x, t)|$.

$$f_0(x,t) = \exp(-x)/x,$$

$$f_1(x,t) = \frac{1}{2}(x-2)\exp(-x)t,$$

$$f_2(x,t) = \frac{1}{12}x(6-6x+x^2)\exp(-x)t^2,$$

$$f_3(x,t) = \frac{1}{144}x^2(-24+36x-12x^2+x^3)\exp(-x)t^3,$$

...

and so on, other components easily obtained by using (27) and MAPLE. A few terms approximation to the solution of Eqs. (22) and (23) can be obtained by setting p = 1 in (28). We get the third-order approximation solution as follows:

$$\bar{f}(x,t) = \sum_{i=0}^{3} f_i(x,t)$$

= $\exp(-x) \left(\frac{1}{x} + \frac{1}{2}(x-2)t + \frac{1}{12}x(6-6x+x^2)t^2 + \frac{1}{144}x^2(-24+36x-12x^2+x^3)t^3 \right).$

Figs. 3 and 4 show that the numerical approximate solution has a high degree of accuracy.

4. Conclusions

In this paper, we used HPM for solving the homogenous Smoluchowski's coagulation equation with constant kernel.

Numerical results obtained show high accuracy of the method as compared with the exact solution. The solution obtained by HPM is valid for not only weakly nonlinear equations but also strong ones. The method gives rapidly convergent successive approximations and handles linear and nonlinear problems in a similar manner.

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