On Solving the Homogeneous Smoluchowski's Equation Utilizing Adomian's Decomposition Method

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ABSTRACT

The Smoluchowski's equation as a partial differential equation models the diffusion and binary coagulation of a large collection of tiny particles. The mass parameter, indexed either by positive integers, or positive reals, corresponds to the discrete or continuous form of the equations. In this article, we try to use the Adomian's decomposition method (ADM) to approximate the solution of the homogeneous Smolochowski's equation. Some test problems have been included to show the accuracy of the method compared with their exact solutions.

KEYWORDS

Adomian's decomposition method, the homogeneous Smoluchowski's equation

1. Introduction

It is a common practice in statistical mechanics to formulate a microscopic model with simple dynamical rules in order to study a phenomenon of interest. In a colloid, a population of comparatively massive particles is agitated by the bombardment of much smaller particles in the ambient environment; the motion of the colloidal particles may then be modeled by Brownian motion [1]. Smoluchowski's equation provides a macroscopic description for the evolution of the cluster densities in a colloid whose particles are prone to binary coagulation. Smoluchowski's equation comes in two flavors: discrete and continuous. In the discrete version, the cluster mass may take values in the set of positive integers, whereas, in the continuous version, the cluster mass take values in $\mathbb{R}^+$. Writing $f_n(x,t)$ for the density of clusters (or particles) of size n, this density evolves according to

$$\frac{\partial f_n(x,t)}{\partial t}=d(n)\Delta f_n(x,t)+Q_+^n(f)(x,t)-Q_-^n(f)(x,t);\ x\in\mathbb{R}^d$$

where

$$Q_+^n(f)=\int_0^n \beta(m,m-n)f_m f_{n-m}dm,$$

$$Q_-^n(f)=2\int_0^\infty \beta(m,n)f_m f_n dm. \qquad (1.1)$$

In which $d(n)\Delta f_n(x,t)$ and $Q_+^n(f)(x,t)-Q_-^n(f)(x,t)$ are respectively diffusion and coagulation parts in the case of the continuous Smoluchowski's equation and $\beta(m,n)$ is considered as a function of the parameters $\alpha(m,n)$(the microscopic coagulation rate), $d(m)$ and $d(n)$. In the discrete case, the integrations given in (1.1) are replaced with summations. In [1] and [2], the discrete Smoluchowski's equation is derived as a microscopic model of coagulating Brownian particles. In this paper we consider the continuous homogenous Smoluchowski's equation. The main purpose of this study is to approximate the solution of continuous homogenous Smoluchowski's equation in which the main technical tool is the Adomian's decomposition method. To our knowledge the problem, so far, has not been considered via ADM and other methods have been performed for only constant kernels [3]. However, the issue of more complicated kernels, which so far have been remained unsolved, will be investigated in our future studies. Let us consider the homogenous Smoluchowski's equation without diffusion part:

$$\frac{\partial}{\partial t}f(x,t)=\frac{1}{2}N_1(f)(x,t)-N_2(f)(x,t), \qquad (1.2)$$

where

$$N_1(f)=\int_0^x k(x-y,y)f(x-y,t)f(y,t)dy, \qquad (1.3)$$

and

$$N_2(f)=\int_0^\infty k(x,y)f(x,t)f(y,t)dy. \qquad (1.4)$$

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where $N_1(f)$ and $N_2(f)$ are nonlinear parts in view of ADM. In the next section, we show how ADM works well.

2. THE DECOMPOSITION METHOD [4]

Eq. (1.1) may be written in the operator form:

$$Lf = N_1(f) - N_2(f), \tag{2.1}$$
$$f(x,0) = f(x),$$

and the differential operator L is

$$L = \frac{\partial}{\partial t}. \tag{2.2}$$

The inverse operator L^{-1} is an integral operator given by

$$L^{-1}(\cdot) = \int_0^t (\cdot)dt. \tag{2.3}$$

Applying L^{-1} upon both sides of (2.1) and using the initial condition, we find

$$f(x,t) = f(x,0) + L^{-1}\left(\frac{1}{2}N_1(f) - N_2(f)\right). \tag{2.4}$$

According to the Adomian's decomposition method the unknown function $f(x,t)$ can be written as

$$f(x,t) = \sum_{n=0}^{\infty} f_n(x,t), \tag{2.5}$$

Substituting (2.5) into the functional equation (2.4) yields

$$\sum_{n=0}^{\infty} f_n(x,t) = f(x) + L^{-1}\left(\frac{1}{2}\sum_{n=0}^{\infty} A_n - \sum_{n=0}^{\infty} B_n\right), \tag{2.6}$$

where $f_0, f_1, \ldots, f_n$ are Adomian's polynomials and the components A_n, B_n 's will be determined recurrently as:

$$A_n = \frac{1}{n!}\frac{d^n}{d\lambda^n}\left[N_1\left(\sum_{i=0}^{\infty}\lambda^i f_i\right)\right]_{\lambda=0}, \quad \text{I}$$

$$B_n = \frac{1}{n!}\frac{d^n}{d\lambda^n}\left[N_2\left(\sum_{i=0}^{\infty}\lambda^i f_i\right)\right]_{\lambda=0}, n = 0,1,2,\ldots. \tag{2.7}$$

It is well known that these polynomials can be constructed for all classes of nonlinearity in view of the algorithms set by Adomian [4] and recently developed by different alternative approaches [5,6]. Thus, we have

$$f_0(x,t) = f(x,0),$$
$$f_{n+1}(x,t) = L^{-1}\left(\frac{1}{2}A_n - B_n\right), \quad n = 0,1,2,\ldots \tag{2.8}$$

Note that the first few components of $f_n(x,t)$ follow immediately upon setting [7]:

$$f_0(x,t) = f(x),$$
$$f_1(x,t) = L^{-1}\left(\frac{1}{2}A_0 - B_0\right),$$
$$f_2(x,t) = L^{-1}\left(\frac{1}{2}A_1 - B_1\right),$$
$$\vdots \tag{2.9}$$

It is, in principle, possible to calculate more components in the decomposition series to enhance the approximation and recursively determine more terms of the series $\sum_{n=0}^{\infty} f_n(x,t)$; hence the solution $f(x,t)$ is readily obtained in a series form as:

$$\phi_n(x,t) = \sum_{k=0}^{n} f_k(x,t), \quad n \geq 0. \tag{2.11}$$

where $\lim_{n\to\infty}\phi_n = f(x,t)$ [8, 9].

Moreover, the decomposition method series (2.11) solutions generally converge very rapidly in real physical problems [9]. The convergence of decomposition series have investigated by several authors [8, 10, and 11], in which they have obtained some results about the speed of convergence of ADM applicable in linear and nonlinear functional equations.

3. APPLICATIONS

In this section the method is applied to some numerical examples with known exact solutions [12].

Example.1: Let us examine the homogenous Smoluchowski's equation (1.2) subject to the initial condition [12]

$$f(x,0) = e^{-x}. \tag{3.1}$$

We compare the numerical solution with the exact available solution of (1.2) [11]. For an arbitrary given $\aleph_0 > 0$, the explicit solution of (1.1) is

$$f(x,t) = \aleph(t)^2 e^{(-\aleph(t)x)} \text{ with } \aleph(t) = \frac{2\aleph_0}{2 + \aleph_0 t}, \tag{3.2}$$

for $(x,t) \in \mathbb{R}_+^2$, where $\aleph(t)$ and $\Re(t)$ defined below are respectively the total number and the total volume of particles .

$$\aleph(t) = \int_0^{\infty} f(x,t)dx,$$
$$\Re(t) = \int_0^{\infty} xf(x,t)dx. \tag{3.3}$$

It is easy to check that $\aleph(t)$ is a non-increasing function of time and $\Re(t)$ might not remain constant throughout time evolution for some coagulation coefficient $k(x,y)$ [12, 13].

Now, consider the equation (1.2)-(1.4) subject to initial condition (3.1) with $k(x,y) = 1$ and $f(x) = \exp(-x)$ [7]. In Figures 1-7, we demonstrate the approximate solutions with different ranges of x and t .

Applying the inverse operator L^{-1} on both sides of (1.1) and using the decomposition series (2.4), (2.5) and (2.6), one gets

$$\sum_{n=0}^{\infty} f_n(x,t) = e^{-x}$$
$$+\frac{1}{2}L^{-1}\int_0^x\left(\sum_{n=0}^{\infty}\lambda^n f_n(x-y,t)\right)\left(\sum_{n=0}^{\infty}\lambda^n f_n(y,t)\right)dy$$
$$-\int_0^{\infty}\left(\sum_{n=0}^{\infty}\lambda^n f_n(x,t)\right)\left(\sum_{n=0}^{\infty}\lambda^n f_n(y,t)\right)dy. \quad (3.4)$$

Proceeding as before, the Adomian's decomposition method [4, 14, 15, and 16] gives the recurrence relations:

$$f_0(x,t) = e^{-x},$$
$$f_1(x,t) = \left(\frac{1}{2}\right)xe^{-x}t - e^{-x}t,$$
$$f_2(x,t) = \left(\frac{1}{2}\right)\left(\frac{1}{4}x(x-4)e^{-x} - \frac{1}{2}xe^{-x} + \frac{3}{2}e^{-x}\right)t^2, \quad (3.5)$$
$$f_3(x,t) = \left(\frac{1}{3}\right)\left(\frac{1}{16}x\left(x^2+20-10x\right)e^{-x} - \frac{1}{8}x^2e^{-x} - \frac{3}{2}e^{-x} + xe^{-x}\right)t^3,$$
$$f_4(x,t) = \left(\frac{1}{4}\right)\left(\frac{1}{96}x\left(-120+90x+x^3-18x^2\right)e^{-x} - \frac{1}{48}x^3e^{-x} - \frac{5}{4}xe^{-x} + \frac{5}{16}x^2e^{-x} + \frac{5}{4}e^{-x}\right)t^4,$$
$$\vdots$$

where A_n, B_n's are Adomian's polynomials that represent the nonlinear terms, given by

$$A_0 = \int_0^x e^{-x+y}e^{-y}dy,$$
$$A_1 = \frac{1}{1!}\frac{d}{d\lambda}\int_0^x\left(e^{-x+y} + \lambda\left(\frac{1}{2}(x-y)e^{-(x-y)}t - e^{-(x-y)}t\right)\right)\left(e^{-y} + \lambda\left(\frac{1}{2}ye^{-y}t - e^{-y}t\right)\right)dy,$$
$$A_2 = \frac{1}{2!}\frac{d^2}{d\lambda^2}\int_0^x\left(e^{-x+y} + \lambda\left(\frac{1}{2}(x-y)e^{-(x-y)}t - e^{-(x-y)}t\right) + \lambda^2\left(\frac{1}{2}\left(\frac{1}{4}(x-y)(x-y-4)e^{-(x-y)} - \frac{1}{2}(x-y)e^{-(x-y)} + \frac{3}{2}e^{-(x-y)}\right)t^2\right)\right)$$
$$\left(e^{-y} + \lambda\left(\frac{1}{2}ye^{-y}t - e^{-y}t\right) + \lambda^2\left(\frac{1}{2}\left(\frac{1}{4}y(y-4)e^{-y} - \frac{1}{2}ye^{-y} + \frac{3}{2}e^{-y}\right)t^2\right)\right)dy,$$
$$\vdots$$

$$B_0 = \int_0^{\infty} e^{-x}e^{-y}dy, \quad (3.6)$$
$$B_1 = \frac{1}{1!}\frac{d}{d\lambda}\int_0^{\infty}\left(e^{-x} + \lambda\left(\frac{1}{2}xe^{-x}t - e^{-x}t\right)\right)\left(e^{-y} + \lambda\left(\frac{1}{2}ye^{-y}t - e^{-y}t\right)\right)dy,$$
$$B_2 = \frac{1}{2!}\frac{d^2}{d\lambda^2}\int_0^{\infty}\left(e^{-x} + \lambda\left(\frac{1}{2}xe^{-x}t - e^{-x}t\right) + \lambda^2\frac{1}{2}\left(\frac{1}{4}x(x-4)e^{-x} - \frac{1}{2}xe^{-x} + \frac{3}{2}e^{-x}\right)t^2\right)$$
$$\left(e^{-y} + \lambda\left(\frac{1}{2}ye^{-y}t - e^{-y}t\right) + \lambda^2\frac{1}{2}\left(\frac{1}{4}y(x-4)e^{-x} - \frac{1}{2}xe^{-x} + \frac{3}{2}e^{-x}\right)t^2\right)dy.$$
$$\vdots$$

Now in view of (3.5), the solution in series form is

$$f(x,t) = e^{-x} + \frac{1}{2}xe^{-x}t - e^{-x}t + \frac{1}{2}\left(\frac{1}{4}x(x-4)e^{-x} - \frac{1}{2}xe^{-x} + \frac{3}{2}e^{-x}\right)t^2$$
$$+\frac{1}{3}\left(\frac{1}{16}x\left(x^2+20-10x\right)e^{-x} - \frac{1}{8}x^2e^{-x} - \frac{3}{2}e^{-x} + xe^{-x}\right)t^3$$
$$+\cdots \quad (3.7)$$

In Figures 1-4, we demonstrate the approximate solutions with different ranges of x and t where the error values at some specific points are presented in Table1.

Example.2: Consider the multiplicative coagulation kernel $k(x,y) = xy$ which has the exact solution [7],

$$f(x,t) = e^{(-T x)}\frac{I_1\left(2xt^{\frac{1}{2}}\right)}{x^2t^{\frac{1}{2}}},$$

subject to the initial condition $f(x,0) = \frac{e^{-x}}{x}$ where

$$T = \begin{cases} 1+t & \text{if } t \le 1, \\ 2t^{1/2} & \text{otherwise.} \end{cases}$$

and I_1 is the modified Bessel function of the first kind

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

As before, ADM gives the recurrence relations:

$$f_0(x,t)=\frac{e^{-x}}{x},$$
$$f_1(x,t)=\frac{1}{2}xe^{-x}t-e^{-x},$$
$$f_2(x,t)=\frac{1}{2}\left(\frac{1}{6}x^2(x-3)e^{-x}-\frac{1}{2}e^{-x}(x-2)x\right)t^2, \qquad (3.8)$$
$$f_3(x,t)=\left(\frac{1}{3}\right)\left(\frac{1}{48}x^3\left(x^2+12-8x\right)e^{-x}-\frac{1}{12}x^2e^{-x}\left(6-6x+x^2\right)\right)t^3,$$
$$f_4(x,t)=\left(\frac{1}{4}\right)\left(\frac{1}{720}x^4\left(-60+60x-15x^2+x^3\right)e^{-x}-\frac{1}{144}x^3e^{-x}\left(-24+36x-12x^2+x^3\right)\right)t^4,$$
$$\vdots$$

Now in view of (3.8), the solution in series form is

$$f(x,t)=\frac{e^{-x}}{x}+\frac{1}{2}xe^{-x}t-e^{-x}+\frac{1}{2}\left(\frac{1}{6}x^2(x-3)e^{-x}-\frac{1}{2}e^{-x}(x-2)x\right)t^2 \qquad (3.9)$$
$$+\left(\frac{1}{3}\right)\left(\frac{1}{48}x^3\left(x^2+12-8x\right)e^{-x}-\frac{1}{12}x^2e^{-x}\left(6-6x+x^2\right)\right)t^3$$
$$+\left(\frac{1}{4}\right)\left(\frac{1}{720}x^4\left(-60+60x-15x^2+x^3\right)e^{-x}-\frac{1}{144}x^3e^{-x}\left(-24+36x-12x^2+x^3\right)\right)t^4$$
$$+\ldots$$

Figures 5-6, illustrate the approximate solutions with different ranges of x and t and the error values at some specific points are presented in Table2. Overall our performed calculations indicate that results obtained via ADM are satisfactory for $x>0$. But, as $x\to 0^{+}$ the computed solution deviates significantly fro the exact solution. Acordingly comparing with [12], for $x>0$ ADM seems to be superior to FDM but as $x\to 0$ the ADM approach is inferior to FDM.

Table1 (Ex.1) for $n=3$

x	t	Numerical Sol	Exact Sol	Error values
1	0.5	0.2872261849	0.2875705370	0.0003443521
2	0.5	0.1291676596	0.1292137715	0.0000461119
5	0.5	0.01171793029	0.01172200889	0.407860e-5
10	0.5	2.154723229e-4	2.146960819e-4	-0.7762410e-7

Table2 (Ex.2) for $n=1$, $n=5$ and $n=10$

x	t	Numerical Sol	Exact Sol	Error values
(n=1)				
1	0.5	0.2835737358	0.2837598582	0.0001861224
2	0.5	0.05638970132	0.05961585954	0.00322615822
(n=5)				
5	0.5	5.162511274e-4	5.21850764e-3	0.00005599637
(n=10)				
10	0.5	6.155335225e-4	6.189432790e-4	3.4097565e-5

4. CONCLUSION

In this paper, we presented a numerical scheme for solving the continuous homogenous Smoluchowski's equation with kernels involving at most two variables x and y. We have approximated $f(x,t)$ by the Adomian's polynomials. Numerical results show high accuracy of the method, as compared with the exact solution. To our knowledge no numerical solution for this problem seems available for comparison.

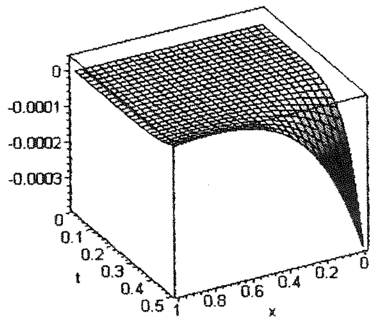

Figure 1 :(Ex.1) The exact error function with $n=5$ and $N_0=1$

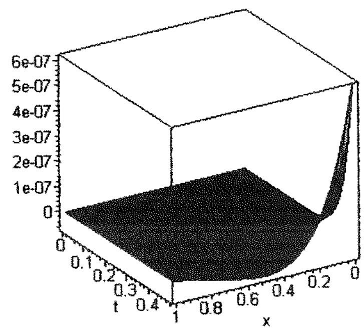

Figure 2 :(Ex.1) The exact error function with $n=10$ and $N_0=1$

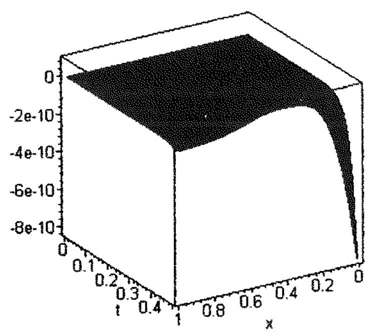

Figure 3 :(Ex.1) The exact error function with $n=15$ and $N_0=1$

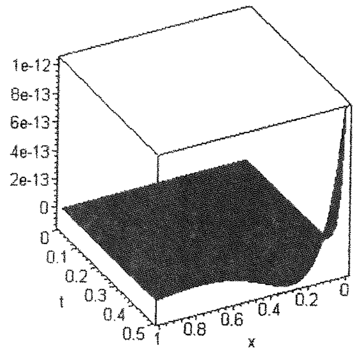

Figure 4 :(Ex.1) The exact error function with $n=20$ and $N_0=1$

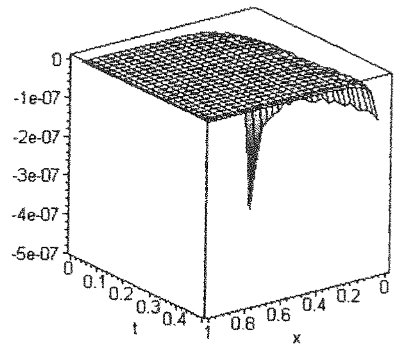

Figure 7 :(Ex.2) The exact error function with $n=10$ and $N_0=1$

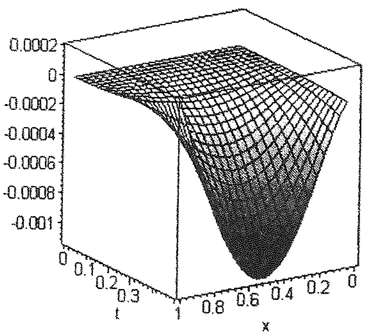

Figure 5 :(Ex.2) The exact error function with $n=1$ and $N_0=1$

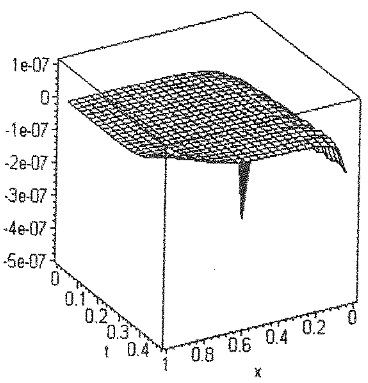

Figure 6 :(Ex.2) The exact error function with $n=5$ and $N_0=1$

4. Reference:

[1] A. Hammond, F. Rezakhanlou. The kinetic limit of a system of coagulating Brownian particles. Archive for Relation *Mechanics and Analysis*, Vol. 185, No. 1. (July 2007), pp. 1-67.

[2] A. Hammond, F. Rezakhanlou. Kinetic limit for a system of coagulating planar Brownian particles. *J. Stat. Phys.* 124 No. 2-4, 997-1040.

[3] M. Ranjbar, H. Adibi, M. Lakestani. Numerical solution of nonlinear ordinary differential equations using Flatlet oblique multiwavelets. International journal of computer mathematics. To appear.

[4] J. Biazar, S. M. Shafiof. A simple algorithm for calculating Adomian polynomials. Int. J. Contemp. Math. Sciences, Vol. 2, (2007), No. 20, 975-982.

[5] Wazwaz AM. A reliable modification of Adomian decomposition method. *Appl Math Comput* 1999; 102: 77-86.

[6] Wazwaz AM. The decomposition for approximate solution of the Goursat problem. Boston (MA): Kluwer Academic Publishers; 1994.

[7] Adomian G. A review of the decomposition method in applied mathematics. *J Math Anal Appl* 1998; 135:501-44.

[8] Y. Cherruault, Convergence of Adomian's method, Kybernetics 18 (1989) 31- 38.

[9] Y. Cherruault, G. Adomian, Decomposition methods: a new proof of convergence, *Math. Comput.* Modeling 18 (1993) 103-106.

[10] F. Filbet, P. Laurencot. Numerical Simulation of Smoluchowski's Coagulation Equation. SIAM J. Sci. Comput. Vol. 25, No. 6, pp. 2004-2008.

[11] Y.C. Jiao, Y.Yamamoto, C.Dong, Y.Hao, An after treatment technique for improving the accuracy of Adomian's decomposition method, *Computers and Mathematics with Applications*, 43, 783-798, (2000).

[12] F. Filbert and Ph. Laurencot. Numerical simulation of the Smoluchowski coagulation equation, *SIAM J. Sci. Comput.* Vol. 25, No. 6, (2004), pp. 2004-2028.

[13] F. Leyvraz and H.R Tschudi, Singularities in the kinetics of coagulation processes, *J. Phys.* A 14, (1981), 3389-3405.

[14] Adomian G. Solving frontier problems of physics: the decomposition method. Boston (MA): Kluwer Academic Publishers; 1994.

[15] Dogan Kaya, Ibrahim E. Inan. A convergence analysis of the ADM and an application. *Applied Mathematics and Computation* Volume 161, Issue 3, (2005) 1015-1025.

[16] Wazwaz AM. A new algorithm for calculating Adomian polynomials for nonlinear operators. *Appl Math Comput* 2000; 111: 53-69.