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New Method for Homogeneous Smoluchowski Coagulation Equation

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Abstract
In this paper, He's Variational iteration method is employed to solve the homogenous Smoluchowski coagulation equation. In statistical physics, the Smoluchowski coagulation equation is a population balance equation, describing the time evolution of the number density of particles as they coagulate to size *x* at time *t*. The intervals of validity of the solutions will be extended by using Pade approximation. Error will be decrease, as it is expected. The numerical results show the effectiveness and the simplicity of the methods.

2010 Mathematics Subject Classification: 45K05, 35Q9.
Key Words and Phrases
Variational Iteration Method, Pade Approximation, Homogenous Smoluchowski Coagulation Equation, Lagrange Multiplier.

1. Introduction

Variational iteration method (VIM) has been proposed by Ji–Huan He, in 1998, and has been applied to solve many linear and non-linear functional equations. There are many research documents, in the literature, for application of VIM to solve different functional equations, such as [1]-[6].

Let us consider the following non-linear functional equation,

$$L\big(u(t)\big)+N\big(u(t)\big)+g(t)=0, \tag{1.1}$$

where L, N and $g(t)$ are a linear, a non-linear operator, and a known analytic function, respectively. In this method, a correction functional including a general Lagrange multiplier, will be constructed as follows,

$$u_{n+1}(t)=u_n(t)+\int_0^t \lambda(s,t)\Big(L\big(u_n(s)\big)+N\big(\tilde{u}_n(s)\big)+g(s)\Big)ds, \quad n\geq 0. \tag{1.2}$$

in which $\tilde{u}_n$ is restricted variations, i.e., $\delta\tilde{u}_n=0.$ Lagrange multiplier can be identify optimally via the variational theory. An iterative formula, for computing the sequence of the approximations, will be obtained as soon as the Lagrange multiplier is determined. The successive approximations $u_n(t),\ n\geq 0,$ of $u(t)$ will be obtained by selection an initial approximation of the solution, u_0. Initial and boundary conditions must be satisfied by initial approximation, u_0. Iterative formula is constructed as follows;

$$u_{n+1}(t)=u_n(t)+\int_0^t \lambda(s,t)\Big(L\big(u_n(s)\big)+N\big(u_n(s)\big)+g(s)\Big)ds, \quad n\geq 0. \tag{1.3}$$

Exact solution will be determined as the following limit,

$$u(t)=\ell im_{n\to\infty}u_n(t).$$

2. Pade Approximation

The series solution obtained by VIM has a small region of convergence. To extend the region of convergence, Pade approximation will be helpful. Pade approximation of a function is given by the ratio of two polynomials [4]. The coefficients of the polynomials in the numerator and denominator are determined by using the coefficients in the Taylor series expansion of the function. The Pade approximation of a function is shown as the following,

$$\left[\frac{m}{n}\right]=\frac{a_0+a_1t+a_2t^2+...+a_mt^m}{b_0+b_1t+b_2t^2+...+b_nt^n}=c_0+c_1t+c_2t^2+...+c_{m+n}t^{m+n}, \tag{2.1}$$

where c_i 's are known coefficients and, a_i 's and b_i 's should be determined. The numerator and denominator have no factors in common.

3. Homogeneous Smoluchowski Coagulation Equation

The physical process of coagulation of particles is often modeled by Smoluchowski's equation. This equation is widely applied to describe the time evolution of the cluster-size distribution during aggregation processes. In this paper, the following Smoluchowski's equation [7], [8], will be considered;

$$\frac{\partial u(x,t)}{\partial t}=C^+(u)-C^-(u), \quad x,t\,\epsilon\mathbb{R}^+, \tag{3.1}$$

$$u(x,0)=u_0, \quad x\epsilon\mathbb{R}^+, \tag{3.2}$$

where:

$$C^+(u)=\frac{1}{2}\int_0^x k(x-y,y)u(x-y,t)u(y,t)\,dy, \tag{3.3}$$

$$C^-(u)=\int_0^\infty k(x,y)u(x,t)u(y,t)\,dy. \tag{3.4}$$

u_0 , is a known function. $u(x,t)$, is the density of cluster of mass x per unit volume at time t . Eq. (3.1) has been used in an amazingly diverse range of applications, such as the formation of clouds and smog [10], the clustering of planets, stars and galaxies [11], the kinetics of polymerization [12] and even the schooling of fishes [13] and the formation of marine snow [14].

4. Applications

To illustrate the ability and the simplicity of the methods two examples are presented.

Example 1. Eqs. (3.1) - (3.4) are considered with constant kernel, $k(x,y)=1$ and $u_0=\exp(-x)$, [7]-[9]:

$$\frac{\partial u(x,t)}{\partial t}=\frac{1}{2}\int_0^x k(x-y,y)u(x-y,t)u(y,t)\,dy-\int_0^\infty k(x,y)u(x,t)u(y,t)\,dy, \tag{3.5}$$

$$u(x,0)=\exp(-x). \tag{3.6}$$

The exact solution is,

$$u(x,t)=N^2(t)\,exp(-N(t)x)\,, \quad x,t\epsilon\mathbb{R}^+, \tag{3.7}$$

with $N(t)=\frac{2M_0}{2+M_0t'}$ and $M_0=1.$

To solve Eq. (3.5), the following correction functional is constructed,

$$u_{n+1} = u_n + \int_0^t \lambda(s)\left((u_n)_s - \frac{1}{2}\int_0^x \tilde{u}_n(x-y,s)\tilde{u}_n(y,s)\,dy + \int_0^\infty \tilde{u}_n(y,s)\tilde{u}_n(x,s)\,dy, \right)ds, \tag{3.8}$$

where λ is general Lagrange multiplier, $\tilde{u}_n$ is considered as restricted variations. To determine the value of λ the following procedure should be followed,

$$\delta u_{n+1} = \delta u_n + \delta\int_0^t \lambda(s)\left((u_n)_s - \frac{1}{2}\int_0^x \tilde{u}_n(x-y,s)\tilde{u}_n(y,s)\,dy + \int_0^\infty \tilde{u}_n(y,s)\tilde{u}_n(x,s)\,dy, \right)ds = 0, \tag{3.9}$$

which is equivalent to,

$$\delta u_{n+1} = \left(1+\lambda(t)\right)\delta u_n + \int_0^t \lambda'(s)\ \delta u_n\, ds = 0. \tag{3.10}$$

Stationary conditions on Eq. (3.10) lead to,

$$1+\lambda(t)=0, \qquad \lambda'(s)=0. \tag{3.11}$$

The Lagrange multiplier is obtained as, $\lambda(s)=-1.$ Having this multiplier the iterative formula (3.8) turns to;

$$u_{n+1} = u_n - \int_0^t \left((u_n)_s - \frac{1}{2}\int_0^x u_n(x-y,s)u_n(y,s)\,dy + \int_0^\infty u_n(y,s)u_n(x,s)\,dy, \right)ds, \tag{3.12}$$

Starting with $u_0(x,t)=u(x,0),$ $u_1(x,t)$ and $u_2(x,t)$ are computed as follows;

$$u_1(x,t) = \left(1+\frac{1}{2}(x-2)\right)\exp(-x),$$

$$u_2(x,t) = \left(1+\frac{1}{144}(72x-144)t + \frac{1}{144}\left(18x^2-108x+108\right)t^2 + \frac{1}{144}\left(36x+x^3-12x^2-24\right)t^3\right)\exp(-x),$$

Other approximations easily obtain by (3.12). The fifth-order iterative solution is considered as the approximate solution. Now, diagonal Pade approximation $\left[\frac{2}{2}\right]$ is calculated as follows;

$$\left[\frac{2}{2}\right] = \exp(-x)\frac{1152x^2-1152x-384x^3+48x^4+\left(144x^3+12x^5-72x^4\right)t+\left(x^6-6x^5+18x^4-24x^3\right)t^2}{1152x^2-1152x-384x^3+48x^4+576+\left(172x^2-1440x-816x^3+576+168x^4-12x^5\right)t+\left(126x^4+x^6-18x^5-408x^3+648x^2-432x+144\right)t^2}.$$

Exact solution, approximate solutions via VIM, and VIM-Pade, and absolute errors of these two methods are plotted in Fig.1.

Example 2. As the second example, Eqs. (3.1) – (3.4) are considered with the multiplicative kernel, $k(x,y)=x\,y$ and $u_0=\exp(-x)/x,$ [7]-[9],

$$\frac{\partial u(x,t)}{\partial t} = \frac{1}{2}\int_0^x (x-y)\ y\,u(x-y,t)u(y,t)\,dy - \int_0^\infty x\,y\,u(x,t)u(y,t)\,dy, \tag{3.13}$$

$$u(x,0) = \frac{\exp(-x)}{x}, \tag{3.14}$$

with the exact solution,

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

where $T = \begin{cases} 1+t, & 0\le t\le 1, \\ 2t^{\frac{1}{2}}, & \textit{otherwise.} \end{cases}$

and I_1 is the modified Bessel function of the first kind,

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

Similar to previous example, Lagrange multiplier is determined as, $\lambda(s) = -1.$ Iterative relation may be constructed as follows,

$$u_{n+1} = u_n - \int_0^t \left((u_n)_s - \frac{1}{2}\int_0^x (x-y)\, y\, u_n(x-y,s)\, u_n(y,s)\, dy + \int_0^{\infty} x\, y\, u_n(y,s)\, u_n(x,s)\, dy, \right) ds. \tag{3.15}$$

Starting with $u_0(x,t) = u(x,0),$ $u_1(x,t)$ and $u_2(x,t)$ are computed as follows;

$$u_1(x,t) = \left(\frac{1}{x} + \frac{1}{2}\frac{(x^2-2x)t}{x} \right)\exp(-x),$$

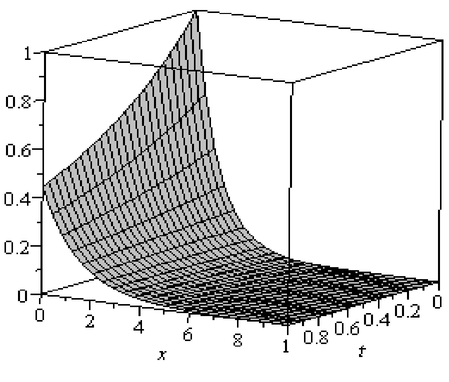
$$u_2(x,t) = \left(\frac{1}{x} + \frac{1}{720}\frac{(360x^2-720x)t}{x} + \frac{1}{720}\frac{(360x^2-360x^3+60x)t^2}{x} + \frac{1}{720}\frac{(20x^4+x^6-10x^5)t^3}{x} \right)\exp(-x),$$

Other approximations will be easily obtained by (3.15). The fourth-order iterative solution is considered as the approximate solution. Now, diagonal Pade approximation $\left[\frac{2}{2}\right]$ can be calculated as follows;

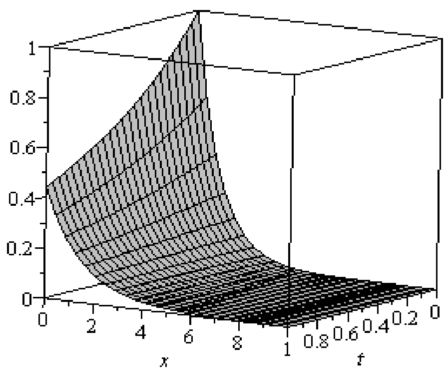
$$\left[\frac{2}{2}\right] = \frac{\exp(-x)}{2}\,\frac{-3600x^3+12960x^2-17280x+8640+360x^4+\left(-11520x^3+10800x^2+6120x^4-1476x^5+138x^6-4320x\right)t+\left(11x^8-138x^7+738x^6-2040x^5-2160x^3+720x^2\right)t^2}{-1800x^4+6480x^3-8640x^2+4320x+180x^5+\left(-1980x^5+5040x^4-5400x^3+2160x^2+342x^6-21x^7\right)t+\left(-660x^6+1260x^5+171x^7-21x^8+x^9-1080x^4+360x^3\right)t^2}.$$

Exact solution, VIM and VIM-Pade approximations, and errors of these two approximations are plotted in Fig. 2.

Fig. 1 Plots of example 1



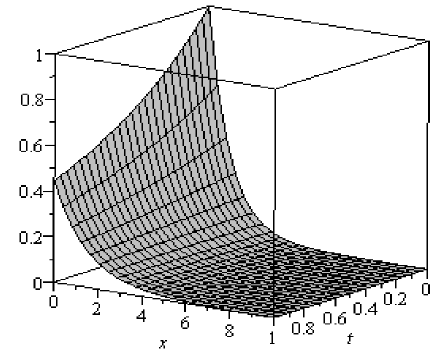
(a)



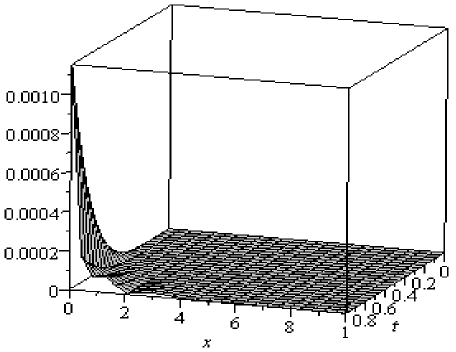
(b)

a: Plot of the exact solution of Example 1

b: Plot of VIM approximation

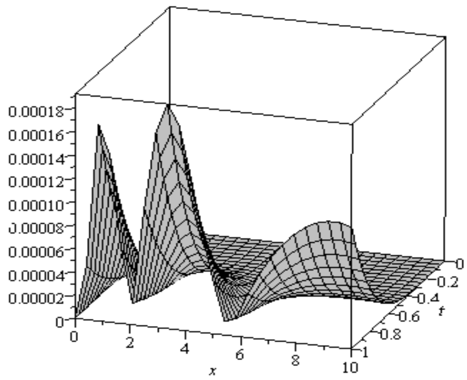


(c)

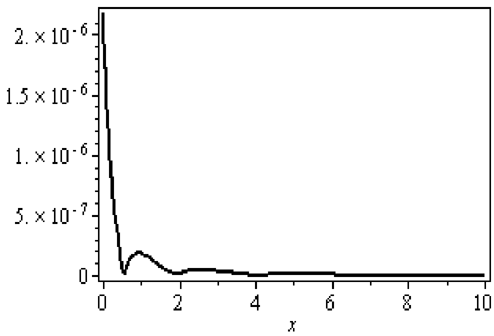


(d)

c: Plot of VIM-Pade approximation
d: Plot of absolute error of VIM approximation

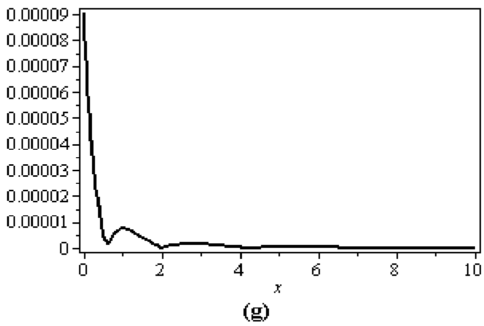


(e)

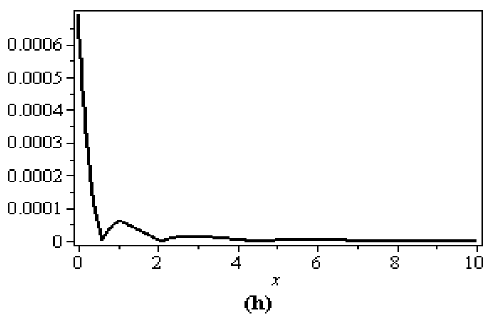


(f)

e: Plot of absolute error of VIM-Pade approximation
f: Plot of absolute error of VIM approximation at time $t = 0.3$

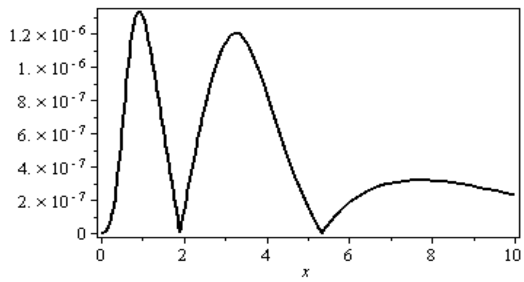


(g)

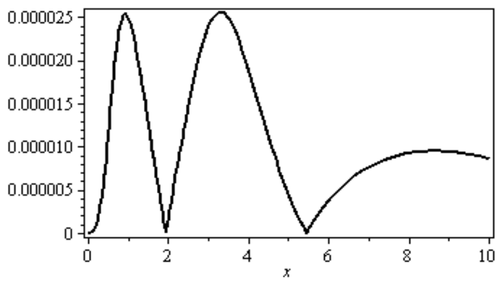


(h)

g: Plot of absolute error of VIM approximation at time $t = 0.6$
h: Plot of absolute error of VIM approximation at time $t = 0.9$

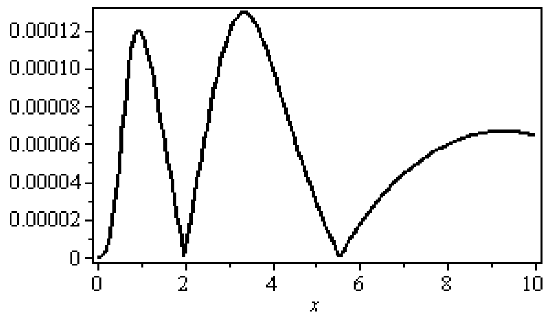


(i)



(j)

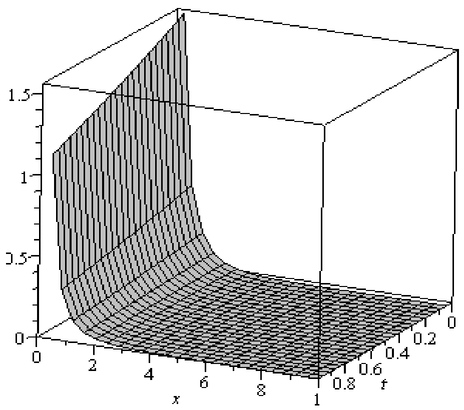
i: Plot of absolute error of VIM-Pade approximation at time $t = 0.3$
j: Plot of absolute error of VIM-Pade approximation at time $t = 0.6$



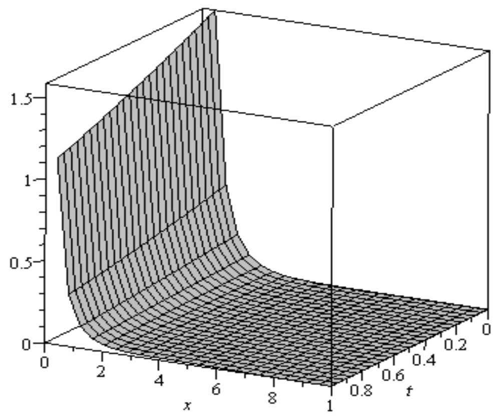
(k)

k: Plot of absolute error of VIM-Pade approximation at time $t = 0.9$

Fig. 2 Plots of example 2

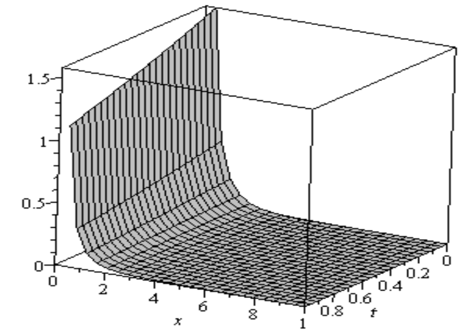


(a)

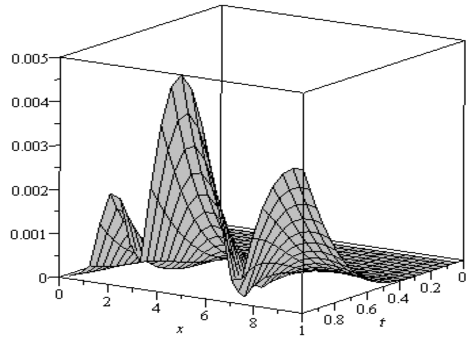


(b)

a: Plot of the exact solution of Example 2
b: Plot of VIM approximation



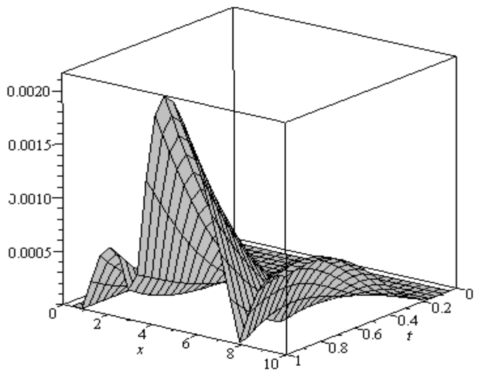
(c)



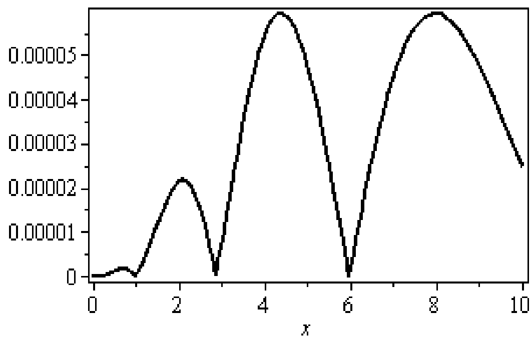
(d)

c: Plot of VIM-Pade approximation

d: Plot of absolute error of VIM approximation

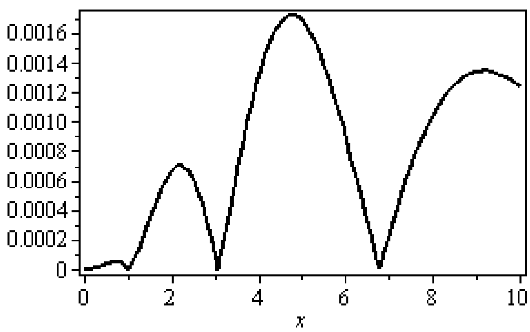


(e)

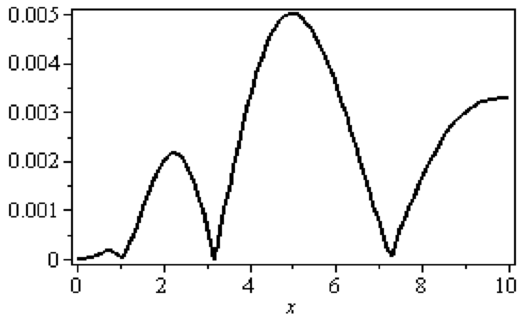


(f)

e: Plot of absolute error of VIM-Pade approximation
f: Plot of absolute error of VIM approximation at time $t = 0.4$

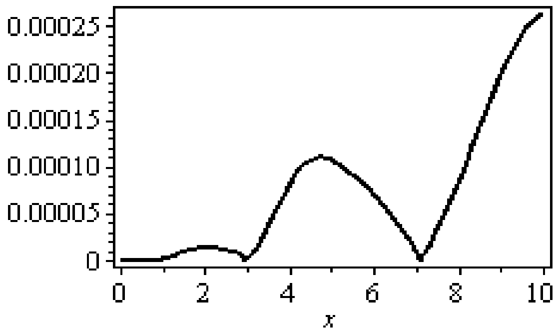


(g)

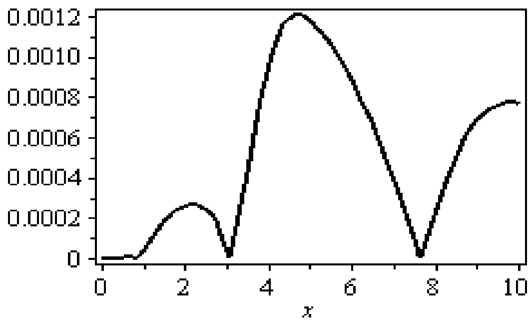


(h)

g: Plot of absolute error of VIM approximation at time $t = 0.8$
h: Plot of absolute error of VIM approximation at time $t = 1$

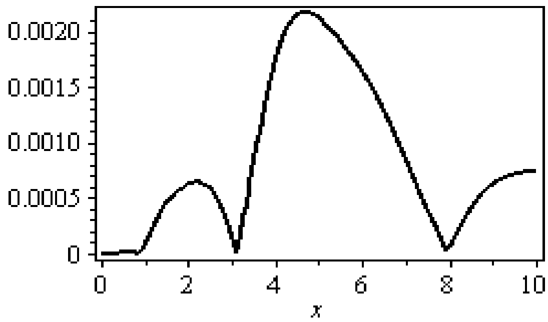


(i)



(j)

i: Plot of absolute error of VIM-Pade approximation at time $t = 0.4$
j: Plot of absolute error of VIM-Pade approximation at time $t = 0.8$



(k)

k: Plot of absolute error of VIM-Pade approximation at time $t = 1$

5. Conclusions

In this paper, Variational iteration method (VIM) and VIM-Pade have been employed to solve the homogeneous coagulation Smoluchowski equation. Obtained solutions have been compared with the exact solutions. Figure 1 and Figure 2 show that the solutions of VIM and VIM-Pade are in good agreement with exact solutions. Also, for two Examples the maximum absolute errors by using of VIM-Pade are lesser than those of VIM. Computations are performed by using the package Maple 13.

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