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Variational Iteration Method for Solving Reaction Diffusion Equation in Oscillatory Chemical Reactions

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ABSTRACT. A mathematical modelling of an oscillatory chemical reactions based on diffusion is discussed. Analytical solutions have been found for the system of nonlinear diffusion equations of second order in the model. Nonlinear oscillation partial differential equations can be solved accurately and efficiently using the He's variational iteration method. He's variational iteration method can be used to obtain approximate analytical solutions to the system. Analytical approximation is compared with numerical simulation as well.

1. Introduction

The periodic property plays a critical role in a variety of oscillatory problems of science and engineering, from oscillations of molecules to earthquakes, as nonlinear oscillations occur everywhere [1-3]. A nanofiber membrane attachment oscillator was developed for controlled manufacturing [4], a water collection oscillator was developed by Fangzhu [5], a harmonic oscillator was developed for micro/nanostructures [6] and a release oscillator was designed for

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delivering ions [7]. Researchers have recently focused attention on nonlinear oscillators, especially after microelectromechanical systems were invented [8-10].

Analytical solutions to oscillation problems are difficult in engineering sciences because most of them are nonlinear. A wide range of physical and chemical sciences have recently examined nonlinear oscillator models. Numerous approximate analytical and numerical methods have been investigated because of the limitations of existing exact solutions. The nonlinear differential equations can be applied to a variety of real-life problems in both pure and applied science [11-13]. This means that analytical/numerical methods are necessary for solving these nonlinear equations. There have been a number of researchers working on analytical methods in the last decade to solve nonlinear oscillation systems [14-16].

A significant amount of computing experience has been gained in the last several years, and certain situations have been analyzed using several numerical methods. Different techniques have been used to develop these approximate analytical methods, including Modified differential transform method [17], Taylor series method [18,19], homotopy perturbation method [20,21], Green function method [22,23], Adomian decomposition method [24], Akbari –Ganji method [25] and variation iteration method [26]. The system of oscillation equations is solved using the variational iteration method in this paper. A wide variety of nonlinear and linear problems arising in various fields have been addressed by He's Variational iteration method [27-29].

The oscillation systems studied by Ganji et al. [30] had nonlinearities such as rigid rod rocking motion. The equations describing nonlinear oscillations of viscoelastic pipelines conveying fluid were developed by Khudayarov and Turaev [31]. As far as we are aware, oscillation problems do not have an exact analytical expression. These problems are difficult to solve precisely, however. An oscillation problem in engineering sciences was analyzed in this paper by obtaining approximate analytical expressions.

2. Mathematical formulation of the problem

A periodic oscillatory chemical reaction in a homogeneous environment has the following kinetic scheme [13]:

$$P_1 \xrightarrow{\lambda_0} X \xrightarrow{\lambda_1} Y \xrightarrow{\lambda_2} P_2 \tag{1}$$

where $\lambda_0, \lambda_1, \lambda_2$ are constant rates and P_1, P_2, X, Y are the concentrations of the corresponding substances. As shown above P_1 reacting with λ_0 to form X, and X reacting with λ_1 to form Y. Finally, Y with λ_2 reacts with P_2.

Considering this chemical reaction as taking place in a very small volume, we can write it as follows

$$X = X(t), Y = Y(t). \tag{2}$$

The equations that describe the reaction are written as differential equations

$$\frac{dX}{dt} = \lambda_0 - \lambda_1 X Y, \tag{3}$$

$$\frac{dY}{dt} = \lambda_1 X Y - \lambda_2 Y, \tag{4}$$

$$\frac{dP_2}{dt} = \lambda_2 Y. \tag{5}$$

The above equations reduced into the form as follows [13]:

$$\frac{\partial x}{\partial t} = -2\delta x - \frac{\omega^2}{2\delta} y + D_1 \frac{\partial^2 x}{\partial u^2}, \tag{6}$$

$$\frac{\partial y}{\partial t} = 2\delta x + D_2 \frac{\partial^2 y}{\partial u^2}. \tag{7}$$

where the coefficients δ and ω are expressed in terms of constant rates.

We solve above differential equations (6) & (7) by taking into account the initial and boundary conditions are as follows:

$$t = 0,\ x = x_0 \cos\left(\frac{n\pi u}{l}\right),\ y = y_0 \cos\left(\frac{n\pi u}{l}\right) \tag{8}$$

$$u = 0,\ \frac{\partial x}{\partial u} = 0,\ \frac{\partial y}{\partial u} = 0, \tag{9}$$

$$u = l,\ \frac{\partial x}{\partial u} = 0,\ \frac{\partial y}{\partial u} = 0. \tag{10}$$

where x_0 and y_0 are constant numbers.

3. Analytical expressions of concentration of the species using variational iteration method

In recent years, several authors have recently demonstrated that the VIM can be effectively used to solve physics and engineering problems with nonlinear structures [32-36]. A boundary value and initial value problem can be defined by the set of expressions in equations (6) & (7). The applicability, accuracy, simple and efficiency of this method make it unique.

Solving the equation (6) and (7) using variational iteration method, we can obtain the concentration of substances for small time as follows:

$$x(u,t) \approx \cos\left(\frac{n\pi u}{l}\right)\left[x_0 - t\left(2\delta x_0 + \frac{\omega^2 y_0}{2\delta} + D_1 \frac{n^2\pi^2 x_0}{l^2}\right)\right] \tag{11}$$

$$y(u,t) \approx \cos\left(\frac{n\pi u}{l}\right)\left[y_0 - t\left(-2\delta x_0 + D_2 \frac{n^2\pi^2 y_0}{l^2}\right)\right] \tag{12}$$

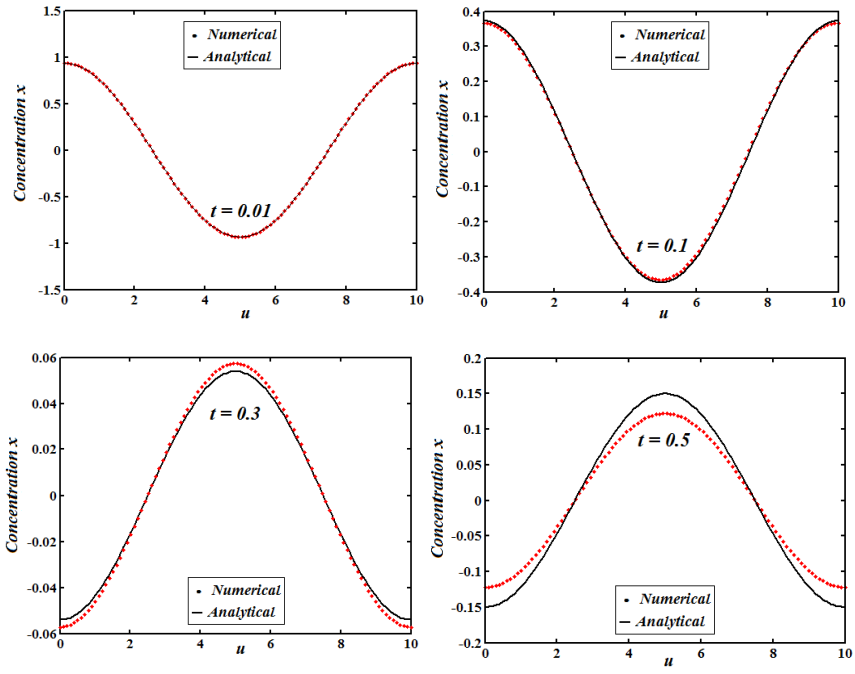

Figure1. Comparison of numerical result with our analytical results using Eq. (11) for the values of $x_0 = 1, y_0 = 1, D_1, D_2 = 1.4\times10^{-5}$, $\omega = 2, \delta = 3, n = 2$ and $l = 10$.

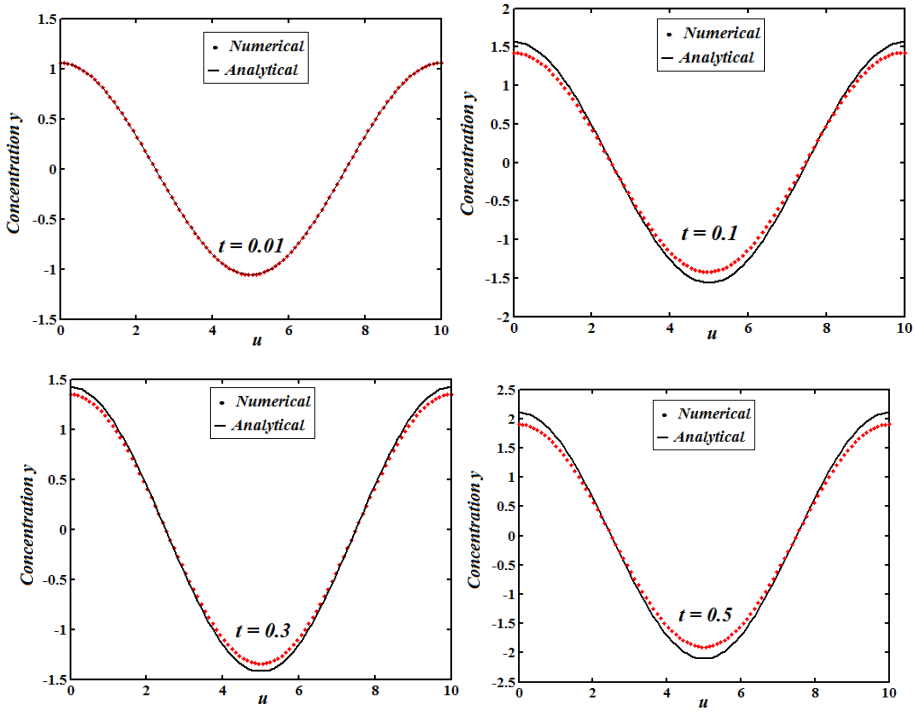

Figure 2. Comparison of numerical result with our analytical results using Eq. (12) for the values of $x_0 = 1, y_0 = 1, D_1, D_2 = 1.4\times10^{-5}$, $\omega = 2, \delta = 3, n = 2$ and $l = 10$.

Table 1. Analyzing the concentration of species x analytically and numerically using Eqn. (11) is compared with the results for different values of t and $x_0 = 1, y_0 = 1, D_1, D_2 = 1.4\times10^{-5}$, $\omega = 2, \delta = 3, n = 2$ and $l = 10$.

x	$t = 0.01$			$t = 0.1$			$t = 0.3$			$t = 0.5$		
	Numerical Result	Our Result	% of deviation	Numerical Result	Our Result	% of deviation	Numerical Result	Our Result	% of deviation	Numerical Result	Our Result	% of deviation
0	0.9352	0.9333	0.20	0.3824	0.3880	1.46	-0.0554	-0.0540	2.44	-0.1409	-0.1500	6.46
2	0.2809	0.2884	2.69	0.1158	0.1191	2.86	-0.0164	-0.0167	1.51	-0.0439	-0.0464	5.50
4	-0.7381	-0.7550	2.30	-0.3100	-0.3139	1.25	0.0436	0.0437	1.29	0.1169	0.1213	3.80
6	-0.7392	-0.7551	2.16	-0.3103	-0.3139	1.17	0.0435	0.0437	0.41	0.1169	0.1214	3.82
8	0.2832	0.2883	1.80	0.1156	0.1198	2.89	-0.0168	-0.0167	0.42	-0.0448	-0.0463	3.33
10	0.9352	0.9333	0.20	0.3823	0.3880	1.49	-0.0554	-0.0540	2.44	-0.1409	-0.1500	6.46
	Average percentage error: 1.56			Average percentage error: 1.76			Average percentage error: 1.94			Average percentage error: 4.89		

Table 2. Analyzing the concentration of species y analytically and numerically using Eqn. (12) is compared with the results for different values of t and $x_0 = 1, y_0 = 1, D_1, D_2 = 1.4\times10^{-5}$, $\omega = 2, \delta = 3, n = 2$ and $l = 10$.

x	$t = 0.01$			$t = 0.1$			$t = 0.3$			$t = 0.5$		
	Numerical Result	Our Result	% of deviation	Numerical Result	Our Result	% of deviation	Numerical Result	Our Result	% of deviation	Numerical Result	Our Result	% of deviation
0	1.0540	1.0325	2.04	1.3820	1.3445	2.71	1.3470	1.3615	1.08	1.9830	2.1026	6.03
2	0.3149	0.3191	1.33	0.4120	0.4093	0.64	0.4081	0.4208	3.11	0.5850	0.6198	5.95
4	-0.8283	-0.8352	0.84	-1.0910	-1.0715	1.79	-1.1100	-1.1015	0.77	-1.6370	-1.7010	3.91
6	-0.8284	-0.8353	0.84	-1.0910	-1.0716	1.77	-1.0790	-1.1016	2.10	-1.5660	-1.6012	2.25
8	0.3148	0.3189	1.30	0.4118	0.4091	0.65	0.4076	0.4206	3.18	0.6798	0.6994	2.89
10	1.0540	1.0325	2.04	1.3870	1.3445	3.06	1.3470	1.3616	1.08	1.9830	2.1026	6.03
	Average percentage error: 1.41			Average percentage error: 1.77			Average percentage error: 1.89			Average percentage error: 4.51		

4. Numerical simulations

Numerical methods are used to solve the nonlinear partial differential equations (6)&(7) with initial and boundary conditions (8)-(10). Using SCILAB/MATLAB software, we can solve this equations (6)&(7) using function pdex4 which solves the initial and boundary value problem. According to Figs 1 and 2, its numerical solution gives satisfactory results for short periods of time when compared with variational iteration method. The SCILAB/MATLAB program is also given in Appendix B.

5. Graphical representation and result Discussion

An approximation of the analytical solution of the system of nonlinear partial differential equations has been compared with numerical result to determine the applicability, accuracy and efficacy of the proposed method.It is used to solve the initial value and boundary value problems using the SCILAB/MATLAB function pdex4 (Fourth order Runge-Kutta method).In Figure 1, shows the numerical solution and an approximate solution we obtained using VIM to demonstrate the concentration versus time for the oscillation problem (Eqs. (11&12)).For various values of the parameter t, the figures 1& 2 shows plot the approximate analytical solution from Equations (11) & (12) using variational iteration method (solid block line) was compared to the computational solution obtained using MATLAB (red dots) for various time t = 0.01, 0.1, 0.3, 0.5. From the figure, it is observed that figure shows a comparison between the numerical solution and our analytical results in Tables 1&2 and Figures 1&2 for a short time when $t \leq 0.5$.The amplitude also depends upon the initial conditions, as shown in Figures 1 and 2. Other nonlinear related ODE/PDE problems can be studied using the present concept as a paradigm.

6. Conclusion

An oscillatory chemical reaction system based on diffusion is constructed and investigated using second order nonlinear partial differential equations.A numerical solution and VIM can also be used to obtain the results. Based on the comparison of approximate analytical solutions with numerical solutions, its accuracy has been verified. In figures, constant parameters are also shown to have an effect on the response of the system for an approximate solution. VIM is a powerful and simple tool for solving nonlinear differential equations, especially those in which nonlinear equations play a large role in science and engineering.

Appendix A: Solution of the Eqs. (6) and (7) using variational iteration method.

To illustrate the basic idea of He's variational iteration method [9-11], we consider the following nonlinear functional equation:

$$Lx(\tau) + Nx(\tau) = g(\tau) \tag{A1}$$

where $Lx(\tau)$ is a linear operator, $Nx(\tau)$ a nonlinear operator and $g(\tau)$ an inhomogeneous term. He et al.[26] suggested a method of general Lagrange multiplier. Then, we can construct a correct functional as follows:

$$x_{n+1}(\tau) = x_n(\tau) + \int_0^{\tau} \lambda(s)\left(Lx_n(\tau) + N\tilde{x}_n(\tau) - g(s)\right)ds, \tag{A2}$$

To solve Eqns.(6) and (7) by variational iteration method, we will have

$$x_{n+1} = x_n + \int_0^{\tau} \lambda_1(s)\left[D_1 \frac{\partial^2 x_n}{\partial u^2} - \frac{\partial x_n}{\partial t} - 2\delta x_n - \frac{\omega^2}{2\delta} y_n \right]ds \tag{A3}$$

$$y_{n+1} = y_n + \int_0^{\tau} \lambda_2(s)\left[D_2 \frac{\partial^2 y_n}{\partial u^2} - \frac{\partial y_n}{\partial t} + 2\delta x_n \right]ds \tag{A4}$$

This yields the stationary conditions

$$\lambda'(s) = 0 \tag{A5}$$

$$1 + \lambda(s)\big|_{s=t} = 0. \tag{A6}$$

Eqn.(A6) is called Lagrange Euler equation, and Eqn. (A6) natural boundary condition.

The general Lagrange multipliers, therefore, can be identified as $\lambda_1(s) = -1$ and $\lambda_2(s) = -1$:

we start with the initial guess $x_0 = a\cos\left(\frac{n\pi u}{l}\right)$, $y_0 = b\cos\left(\frac{n\pi u}{l}\right)$ in the above iteration

When n=0, in Eqn. (A3)

$$x_1 = x_0 - \int_0^{\tau}\left[D_1 \frac{\partial^2 x_0(u,s)}{\partial u^2} - \frac{\partial x_0(u,s)}{\partial s} - 2\delta x_0(u,s) - \frac{\omega^2}{2\delta} y_0(u,s) \right]ds \tag{A7}$$

$$x_1(u,t) = \cos\left(\frac{n\pi u}{l}\right)\left[x_0 - t\left(2\delta a + \frac{\omega^2 b}{2\delta} + D_1 \frac{n^2\pi^2 a}{l^2} \right)\right] \tag{A8}$$

When n=0, in Eqn. (A4)

$$y_1 = y_0 - \int_0^{\tau}\left[D_2 \frac{\partial^2 y_0(u,s)}{\partial u^2} - \frac{\partial y_0(u,s)}{\partial t} + 2\delta x_0(u,s) \right]ds \tag{A9}$$

$$y_1(u,t) \approx \cos\left(\frac{n\pi u}{l}\right)\left[b - t\left(-2\delta a + D_2 \frac{n^2\pi^2 b}{l^2}\right)\right] \quad \text{(A10)}$$

Appendix B: Matlab program for the numerical solution of nonlinear Eqns. (6) and (7)

```
function pdex4
m = 0;
x = linspace (0,10);
t= linspace (0,0.01);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,2)')
figure
plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
ylabel('u2(x,2)')
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
D1=1;
D2=1;
f = [D1; D2] .* DuDx;
q=3;
w=2;
F = -2*q*u(1)-(w^2/(2*q))*u(2);
F1 =2*q*u(1);
s=[F;F1];
function u0 = pdex4ic(x)
```

```
x0=1;y0=1;n=2;l=10;pi=3.1415;
u0 = [x0*(cos(((n*pi)/l)*x));y0*(cos(((n*pi)/l)*x))];
function[pl,ql,pr,qr]=pdex4bc(xl,u1,xr,ur,t)
pl = [0; 0];
ql = [1; 1];
pr = [0; 0];
qr = [1; 1];
```

NOMENCLATURE and UNITS

Symbols	Name	Unit
x	Concentration of species X	$mol\,cm^{-3}$
y	Concentration of species Y	$mol\,cm^{-3}$
P_1, P_2, X, Y	concentrations of the substances	$mol\,cm^{-3}$
$\lambda_0, \lambda_1, \lambda_2$	Constant rates	cm/s
$2\delta = \frac{\omega^2}{\lambda_2},\ \lambda_1\lambda_0 = \omega^2$	Constant rates	cm/s
D_1, D_2	Diffusion coefficient	cm^2/s
u	Spatial coordinate	cm
t	time	s
l	Narrow tube length	cm
n ,a and b	Constant numbers	None

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