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Analytical Solutions of simultaneous Linear Differential Equations in Chemical Kinetics And Homotopy Perturbation Method.

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ABSTRACT: *Analytical method for solving homogeneous linear differential equations in chemical kinetics and pharmacokinetics using homotopy perturbation method has been proposed. The mathematical model that depicts the pharmacokinetics is solved. Herein, we report the closed form of an analytical expression for concentrations species for all values of kinetic parameters. These results are compared with numerical results and are found to be in satisfactory agreement. The obtained results are valid for the whole solution domain.*

Keywords: *Mathematicalmodelling;Linear differential equation; Chemical kinetics; Reaction mechanics;Pharmacokinetics model; Homotopy perturbation method.*

I. INTRODUCTION

Various asymptotic methodis used to solve the linear and nonlinear problem in physical and chemical sciences. Variational iteration methodis a powerful method which yields convergent series solution for linear/nonlinear problems [1]. Also it is a powerful mathematical tool to solving systems of ordinary differential equations. Recently ElhamSalehpoor et.al [2] used the variational iteration method to systems of linear/non-linear ordinary differential equations, which yields a series solution with accelerated convergence.Matinfar et.al [3] proposed VIMHP to solve effectively, easily and accurately a large class of linear, nonlinear, partial,deterministic or stochastic differential equations with approximate solutions whichconverge very rapidly to accurate solutions. Matinfaret.al[4] develop the modified variational iteration method for solving linear problems.

He's homotopy perturbation method is a powerful and capable method to solve linear and nonlinear equation directly. Most of the scientific problems in engineering are linear or nonlinear. Except in a limited number of these problems, finding the exact analytical solutions of such problems are quite difficult. Therefore, there have been attempts to develop new techniques for obtaining analytical solutions which reasonably approximate the exact solutions. Homotopy perturbation method is such method which is straightforward and convenient for both linear and non-linear equations. It is also applicable to both partial differential equation and ordinary differential equation. The homotopy perturbation method is proposed by He in 1999 and was developed and improved by him. Homotopy perturbation method is the combination of traditional perturbation method and homotopy method so it takes full advantages of both methods.In this paper approximate solution of system of linear differential equations in pharmacokinetics model are obtained by Homotopy perturbation method.

II. MATHEMATICAL FORMULATION OF THE PROBLEM

The systematic diagram of pharmacokinetics model for fluoxetine and norfluoxetine is represented in Fig 1.The concentrations of A,B,C,D species with *X, Y, Z* and W can represented by the following system of linear differential equations.

$$\frac{dX}{dt} = -(k_{01} + k_{02})X \quad (1)$$

$$\frac{dY}{dt} = k_{01}X - (k_{10} + k_{12} + k_{13})Y + k_{31}Z \quad (2)$$

$$\frac{dZ}{dt} = k_{13}Y - k_{31}Z \quad (3)$$

$$\frac{dW}{dt} = k_{02}X + k_{12}Y - k_{20}W \quad (4)$$

where$X$ is a concentration of fluoxetine at administration place. Y is a concentration of fluoxetine in central compartment. Z is a concentration of fluoxetine in peripheral compartment and W is a concentration of norfluoxetine in central compartment. The rate coefficients are: k_{01} absorption rate constant for fluoxetine, k_{02} and k_{12} presystematic and systematic metabolism rate constant of fluoxetine to norfluoxetine, k_{13} and k_{31} the distribution rate constants for fluoxetine, k_{10} and k_{20} the elimination rate constants for fluoxetine and norfluoxetine.The initial conditions are

$$X(0) = X_0, Y(0) = Z(0) = W(0) = 0 \quad (5)$$

III. APPROXIMATE ANALYTICAL EXPRESSION FOR CONCENTRATIONS SPECIES USING THE HOMOTOPY PERTURBATION METHOD (HPM)

Some nonlinear problems in chemical sciences [4] can be solved HPM [5], ADM [6, 7] and VIM [8]. Recently, many authors have applied the Homotopy perturbation method (HPM) to solve the linear and non-linear problem in physics and engineering sciences [9-16]. This method is also used to solve some of the non-linear problem in physical sciences [14-16]. This method is a combination of Homotopy in topology and classic perturbation techniques. [2, 17-19] HPM is unique in its applicability, accuracy and efficiency. The HPM uses the imbedding parameter p as a small parameter, and only a few iterations are needed to solve the equation. The basic concept of HPM is given in Appendix A .By solving the Eqns. (1) - (4) using this method [9-11], we can obtain concentrations ofspecies as follows(Appendix B):

$$X(t) = X_0 e^{-at} \quad (6)$$

$$Y(t) = \left[\frac{k_{01}X_0}{b-a}\right]e^{-at} + \left[\frac{k_{31}\varepsilon}{b-k_{31}}\right]e^{-K_{31}t} - \left[\frac{k_{01}X_0}{b-a} + \frac{k_{31}\varepsilon}{b-k_{31}}\right]e^{-bt}$$

$$Z(t) = \left[\frac{k_{13}k_{01}X_0}{(k_{31}-b)(k_{31}-a)}\right]e^{-k_{31}t} + \frac{k_{13}k_{01}X_0}{b-a}\left[\frac{e^{-bt}}{b-k_{31}} - \frac{e^{-at}}{a-k_{31}}\right] \quad (8)$$

$$W(t) = \left[\frac{-k_{02}X_0}{k_{02}-a} + \frac{k_{12}k_{01}X_0}{(k_{20}-b)(k_{20}-a)}\right]e^{-k_{20}t} + \frac{k_{20}X_0e^{-at}}{k_{20}-a} + \frac{k_{12}k_{01}X_0}{b-a}\left[\frac{-e^{-bt}}{k_{20}-b} + \frac{e^{-at}}{k_{20}-a}\right]$$

(9)

where

$$a = k_{01} + k_{02} \text{ and } b = k_{10} + k_{12} + k_{13} \quad (10)$$

IV. NUMERICAL SIMULATION

The linear differential equations (1)-(4) for the given initial conditions are solved by using homotopy perturbation methods. The function pdex 4 in Matlab software, which is a function of solving initial value problems was used to solve these equations numerically and the Matlab program is given in Appendix C. Figures 2-5, and Tables 1-4represent the comparison of analytical results obtained in this work with the numerical results. Upon comparison, it is evident that both the results are in good agreement for different values of the reaction and diffusion parameters.The maximum relative error between our analytical results and simulation results is 0.5%.

V. RESULT AND DISCUSSIONS

Figures 2(a) and 2(b) represents the dimensionless concentration of fluoxetine at administration place$x$ for different values of dimensionless parameter k_{01} and k_{02} .From these figures, it is evident that the values of

the concentrationfluoxetine at administration place decreases when dimensionless time increases and the parameters k_{01} and k_{02} increases. Concentration *X*is a decreasing function of time *t.*

Figures (3(a-c)) represents the dimensionless concentrationof fluoxetine in central compartment*Y* for different values of dimensionless parameters k_{10}, k_{12} and k_{13}.From these Figures,it is evident that the values of the concentration decreases when dimensionless parameters k_{10}, k_{12} and k_{13} increases.Also the concentration *Y* increase gradually from its initial value and reaches the maximal value when time *t*=0.2 for all values of parameter and then concentration decrease from the maximumvalue.

Figure (4) represents the dimensionless concentration of fluoxetine in peripheral compartment Z for different values of dimensionless parameter k_{31}.From these figures, it is evident that the values of the concentration decreases when dimensionless parameters K_{31} increases.

Figure (5) represents the dimensionless concentrationofnorfluoxetine in central compartment *W*for different values of dimensionless parameter k_{20}.From these figures, it is observed that the values of the concentration decreases when dimensionless parameters k_{20} increases. Also the concentration *W*increases from its initial value and reaches maximal value when *t*=0.15 and then decreases gradually and reaches the steady state value when time *t*=1.

VI. CONCLUSION

Approximate analytical solutions of system of linear differential equations in parametric kinetics are presented using homotopy perturbation method. A simple, straight forward and a new method ofestimating the concentrations of species X, Y, Z and W are derived. The primary result of this work is simple approximate calculations of concentration for all values of dimensionless parameters. This solution procedure can be easily extended to solve all kinds of system of coupled linear and nonlinear equations with various complex boundary conditions in chemical and physical sciences.

APPENDIX A

Basic concept of the Homotopy perturbation method (HPM) [9-12]

To explain this method, let us consider the following function:

$$D_o(u) - f(r) = 0, \quad r \in \Omega \quad \text{(A.1)}$$

with the boundary conditions of

$$B_o(u, \frac{\partial u}{\partial n}) = 0, \quad r \in \Gamma \quad \text{(A.2)}$$

where D_o is a general differential operator, B_o is a boundary operator, $f(r)$ is a known analytical function and Γ is the boundary of the domain Ω. In general, the operator D_o can be divided into a linear part L and a non-linear part N. The eqn. (A.1) can therefore be written as

$$L(u) + N(u) - f(r) = 0 \quad \text{(A.3)}$$

By the Homotopy technique, we construct a Homotopy $v(r, p) : \Omega \times [0,1] \to \Re$ that satisfies

$$H(v, p) = (1-p)[L(v) - L(u_0)] + p[D_o(v) - f(r)] = 0. \quad \text{(A.4)}$$

$$H(v, p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0. \quad \text{(A.5)}$$

Where$p \in [0, 1]$ is an embedding parameter, and u_0 is an initial approximation of eqn. (A.1) that satisfies the boundary conditions. From eqns. (A.4) and (A.5), we have

$$H(v,0) = L(v) - L(u_0) = 0 \quad \text{(A.6)}$$

$$H(v,1) = D_o(v) - f(r) = 0 \quad \text{(A.7)}$$

When *p*=0, the eqns. (A.4) and (A.5) become linear equations. When *p* =1, they become non-linear equations. The process of changing *p* from zero to unity is that of $L(v) - L(u_0) = 0$ to $D_o(v) - f(r) = 0$. We first use

the embedding parameter p as a "small parameter" and assume that the solutions of eqns. (A.4) and (A.5) can be written as a power series in p :

$v = v_0 + pv_1 + p^2 v_2 + \ldots$ (A.8)

Setting $p = 1$ results in the approximate solution of the eqn. (A.1):

$u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + \ldots$ (A.9)

This is the basic idea of the HPM.

APPENDIX B

Solution of the eqn. (2)-(4) using the Homotopy perturbation method.

To find the solution of the equations (2) – (4), we construct a Homotopy for the equation(2) as follows:

$$(1-p)\left[\frac{dY}{dt} - k_{01}X + \left[(k_{10}+k_{12}+k_{13})\,Y_0\right]\right] + p\left[\frac{dY}{dt} - k_{01}X + (k_{10}+k_{12}+k_{13})Y - k_{31}Z\right] = 0 \quad \text{(B.1)}$$

Comparing the coefficient of p on both sides

$$\mathrm{P}^{0:}\ \frac{dY_0}{dt} = k_{01}X - \left[(k_{10}+k_{12}+k_{13}).Y_0\right] = 0 \quad \text{(B.2)}$$

Using the initial condition (5),the solution of the above equation becomes

$$Y_0(t) = \frac{k_{01}X_0}{b-a}\left(e^{-at} - e^{-bt}\right) \quad \text{(B.3)}$$

where $a = k_{01} + k_{02}$ and $b = k_{10} + k_{12} + k_{13}$ (B.4)

Substituting $Y(t)$ in the equation (3), we get

$$Z(t) = \left[\frac{k_{13}k_{01}X_0}{(k_{31}-b)(k_{31}-a)}e^{-k_{31}t}\right] + \frac{k_{13}k_{01}X_0}{b-a}\left[\frac{-e^{-bt}}{-b+k_{31}} + \frac{e^{-at}}{-a+k_{31}}\right] \quad \text{(B.5)}$$

Substituting theX(t) and Y(t) in equation (4) ,we get

$$W(t) = \left[\frac{-k_{02}X_0}{k_{02}-a} + \frac{k_{12}k_{01}X_0}{(k_{20}-b)(k_{20}-a)}\right]e^{-k_{20}t} + \frac{k_{20}X_0e^{-at}}{k_{20}-a} + \frac{k_{12}k_{01}X_0}{b-a}\left[\frac{-e^{-bt}}{k_{20}-b} + \frac{e^{-at}}{k_{20}-a}\right]$$

Again substituting *X*and *Z* in the below equation

$$\frac{dY}{dt} = k_{01}.X - (k_{10}+k_{12}+K_{13}).Y + k_{31}.Z \quad \text{(B.7)}$$

we get

$$Y(t) = \frac{k_{01}X_0e^{-at}}{b-a} + \frac{k_{31}\varepsilon e^{-k_{31}t}}{b-k_{31}} - \left[\frac{k_{01}X_0}{b-a} + \frac{k_{31}\varepsilon}{b-k_{31}}\right]e^{-bt} \quad \text{(B.8)}$$

APPENDIX C

Matlab program to find the numerical solution of the equations (1)-(4).

```
function
options= odeset('RelTol',1e-6,'Stats','on');
Xo = [1;0;0;0];
tspan = [0,1];
tic
[t, X] = ode45(@Test Function, tspan, Xo, options);
toc
figure
```

```
holdon
%plot(t, X(:,1))
plot(t, X(:,2))
%plot(t, X(:,3))
%plot(t, X(:,4))
return
function [dx_dt]= TestFunction(t, x)
k01=3;k02=3.3;k10=30;k12=2.2;k13=2.4;k31=0.2;k20=0.6;
dx_dt(1)=-(k01+k02)*x(1);
dx_dt(2)=k01*x(1)-(k10+k12+k13)*x(2)+k31*x(3);
dx_dt(3)=k13*x(2)-k31*x(3);
dx_dt(4)=k02*x(1)+k12*x(2)-k20*x(4);
dx_dt = dx_dt';
return
```

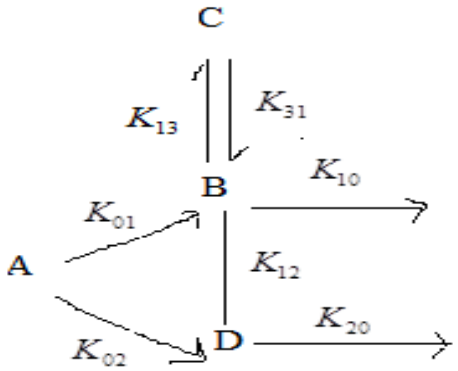

Fig. 1. Pharmacokinetics model for fluoxetine and norfluoxetine [1].

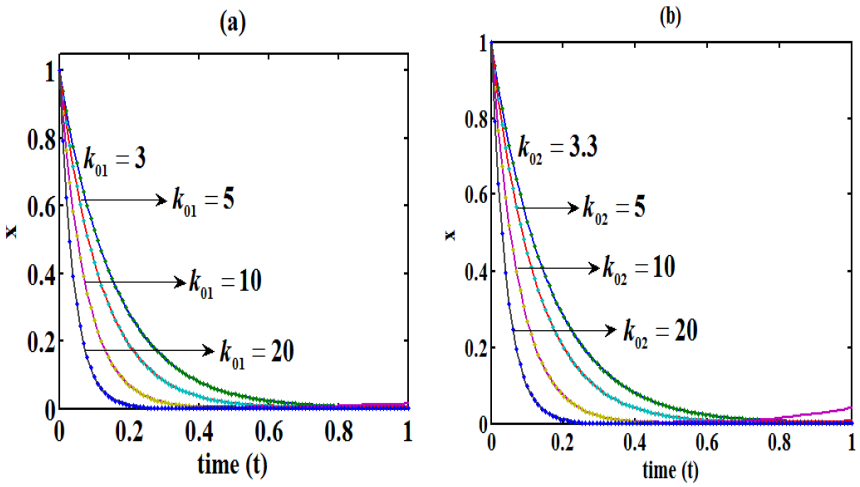

Fig. 2. Comparison between analytical expression of concentration of *X*and numerical results for various values of parameters (a) K_{01} and (b) k_{02}. The key to the graph: solid line represents analytical Eq. (5)and dotted line represent the numerical solution.

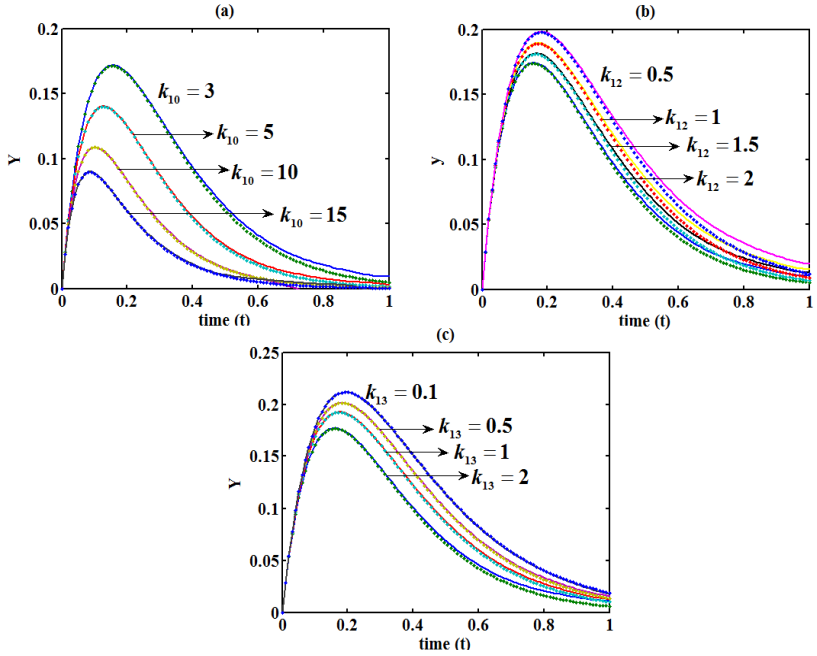

Fig. 3.(a)-(c)Comparison between analytical expression of concentration of Y and numerical results for various values of (a) k_{10} (b) k_{12} and(c) k_{13}. The key to the graph: solid line represents analytical expressionEq. (6)and dotted line represent the numerical solution.

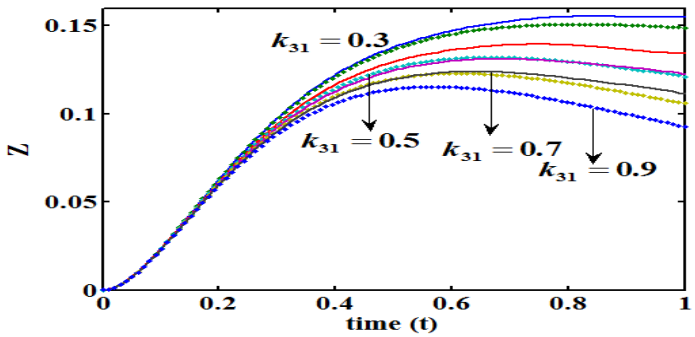

Fig. 4. Comparison between analytical expression of concentration of Z and numerical results for various values of k_{31}. The key to the graph: solid line represents analytical expressionEq. (7) and dotted line represent the numerical solution.

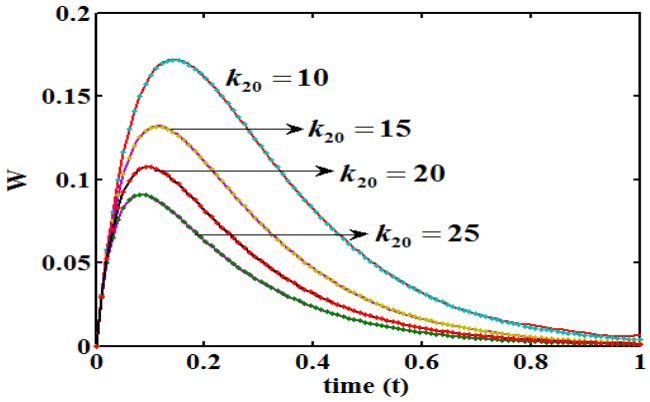

Fig. 5. Comparison between analytical expression of concentration of W and numerical results for various values of k_{20}. The key to the graph: solid line represents analytical expressionEq. (8)and dotted line represent the numerical solution.

Table1: Comparison of analytical expression of concentration of species Y (Eq.(6))with numerical results for various values of parameter k_{10} and the other parametersare $k_{01}=3,\ k_{02}=3.3, k_{12}=2.2, k_{13}=2.4$ and $k_{31}=0.2$.

Time (t)	$k_{10}=3$			$k_{10}=5$			$k_{10}=10$			$k_{10}=15$		
	Numerical	Analytical Eq. (6)	Error%	Numerical	Analytical Eq. (6)	Error%	Numerical	Analytical Eq. (6)	Error%	Numerical	Analytical Eq. (6)	Error%
0.1	0.165821	0.165503	0.191859	0.15775	0.157405	0.21899	0.150213	0.149828	0.256199	0.143171	0.142735	0.304748
0.15	0.185243	0.184419	0.444904	0.171887	0.171029	0.499191	0.159812	0.158909	0.564653	0.148897	0.147925	0.652825
0.2	0.183939	0.182682	0.682966	0.166352	0.165188	0.699687	0.15094	0.149867	0.711188	0.137407	0.136419	0.719027
0.25	0.171457	0.169669	1.042579	0.151101	0.149577	1.008804	0.133824	0.132552	0.950699	0.119087	0.118074	0.850397
0.3	0.153816	0.151296	1.638898	0.132131	0.130026	1.592746	0.114318	0.112587	1.514026	0.09959	0.098215	1.381304
	Average error %		0.800241	Average error %		0.803884	Average error %		0.799353	Average error %		0.781660

Table 2: Comparison ofanalytical expression of concentration of species (Eq.(6))with numerical results for various values of parameter k_{12} and the other parameters are $k_{01}=3, k_{10}=3, k_{13}=2.4$ and $k_{31}=0.2$.

Time (t)	$k_{12}=0.5$			$k_{12}=1$			$k_{12}=1.5$			$k_{12}=2$		
	Numerical	Analytical Eq. (6)	Error %	Numerical	Analytical Eq. (6)	Error %	Numerical	Analytical Eq. (6)	Error %	Numerical	Analytical Eq. (6)	Error %
0.1	0.159328	0.158982	0.217612	0.151674	0.151304	0.244498	0.144543	0.144116	0.295305	0.137886	0.137385	0.363276
0.15	0.174469	0.173601	0.497542	0.162122	0.161238	0.545054	0.150997	0.150037	0.635778	0.140926	0.139874	0.746478
0.2	0.169716	0.168502	0.715335	0.153851	0.152772	0.701295	0.139978	0.138972	0.718561	0.127779	0.126836	0.738104
0.25	0.154957	0.153331	1.049163	0.137045	0.135738	0.953966	0.121845	0.120788	0.867418	0.108875	0.108037	0.768983
0.3	0.136201	0.133946	1.655523	0.117597	0.115808	1.521181	0.102294	0.100875	1.387477	0.089647	0.088516	1.262132
	Average error %		0.827035	Average error %		0.793194	Average error %		0.780907	Average error %		0.775394

Table 3: Comparison of analytical expression of concentration of species Y (Eq.(6)) with numerical results for various values of parameter k_{13} and the other parameters are $k_{01}=3$, $k_{10}=3$, $k_{12}=2.2$ and $k_{31}=0.2$.

Time (t)	$k_{13}=0$			$k_{13}=0.5$			$k_{13}=1$			$k_{13}=2$		
	Numerical	Analytical Eq. (6)	Error %	Numerical	Analytical Eq. (6)	Error %	Numerical	Analytical Eq. (6)	Error %	Numerical	Analytical Eq. (6)	Error %
0.1	0.16077	0.160579	0.216508	0.15313	0.152799	0.216508	0.145983	0.145516	0.319671	0.139308	0.138696	0.43919
0.15	0.176698	0.176224	0.267792	0.164402	0.163614	0.479488	0.153268	0.15219	0.703326	0.143185	0.141829	0.947294
0.2	0.17242	0.171906	0.297996	0.15669	0.155755	0.596953	0.142858	0.141591	0.886956	0.130676	0.129142	1.173915
0.25	0.157775	0.157213	0.356471	0.140137	0.139029	0.790259	0.125076	0.123589	1.189324	0.112179	0.11043	1.558972
0.3	0.138812	0.138025	0.56727	0.120675	0.119156	1.258447	0.105658	0.103637	1.912203	0.093171	0.090807	2.536506
	Average error %		0.3402934	Average error %		0.6683331	Average error %		0.9988168	Average error %		1.3311754

Table 4: Comparison ofanalytical expression of concentration of species Z(Eq. (7))with numerical results for various values of parameter k_{31} and the other parameters are $k_{01}=3, k_{02}=3.3, k_{10}=3, k_{12}=2.2,\ k_{13}=2.4$ and $k_{20}=0.6$.

Time(t)	$k_{31}=0.3$			$k_{31}=0.5$			$k_{31}=0.7$			$k_{31}=0.9$		
	Numerical	Analytical Eq. (7)	Error %	Numerical	Analytical Eq. (7)	Error %	Numerical	Analytical Eq. (7)	Error %	Numerical	Analytical Eq. (7)	Error %
0.1	0.023412	0.023437	0.10855	0.023248	0.023265	0.07271	0.023086	0.023095	0.03717	0.022925	0.022927	0.0063
0.15	0.042881	0.042907	0.0608	0.042424	0.042412	0.027787	0.041974	0.041925	0.115814	0.041529	0.041447	0.197455
0.2	0.062561	0.062426	0.215975	0.061661	0.061422	0.387909	0.06078	0.06044	0.559143	0.059913	0.059481	0.722062
0.25	0.080674	0.080302	0.462307	0.0792	0.078616	0.737609	0.077764	0.076977	1.011679	0.076358	0.075385	1.274765
0.3	0.0964	0.095773	0.650082	0.094243	0.093257	1.046829	0.092156	0.090828	1.441298	0.090124	0.088482	1.821297
	Average error %		0.2258028	Average error %		0.4254848	Average error %		0.5512468	Average error %		0.8018558

Table 5: Comparison of analytical expression of concentration of species W (Eq.(8))with numerical results for various values of parameter k_{20} and the other parameters are $k_{01}=3, k_{02}=3.3, k_{10}=3, k_{12}=2.2,\ k_{13}=2.4$ and $k_{31}=0.2$.

Time (t)	$k_{20}=10$			$k_{20}=15$			$k_{20}=20$			$k_{20}=25$		
	Numerical	Analytical Eq. (8)	Error %	Numerical	Analytical Eq. (8)	Error %	Numerical	Analytical Eq. (8)	Error %	Numerical	Analytical Eq. (8)	Error %
0.1	0.162577	0.162341	0.145229	0.131139	0.130659	0.366051	0.107624	0.10725	0.347231	0.090293	0.08968	0.679368
0.15	0.171929	0.171464	0.27086	0.126838	0.126661	0.139439	0.09732	0.097527	0.21244	0.077435	0.077885	0.58104
0.2	0.161453	0.161356	0.060026	0.11050 4	0.11085	0.31378	0.081147	0.081495	0.42847	0.062713	0.063307	0.946567
0.25	0.142365	0.142663	0.2089	0.091839	0.092203	0.39633	0.065645	0.065597	0.071778	0.05029	0.050141	0.296693
0.3	0.120978	0.121331	0.29205	0.07454	0.074503	0.048738	0.05216	0.051798	0.694834	0.039894	0.039221	1.686395
	Average error %		0.00496	Average error %		0.05655	Average error %		0.09459	Average error %		0.22697

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