

Rach Adomian Decomposition Method to Solve Nonlinear Equations of Chemical Kinetic System

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Abstract: In this research paper, we solved the chemical kinetic system of nonlinear ordinary differential equations by the Modified Adomian i.e. Rach Adomian Decomposition Method (RADM). Rach Adomian Decomposition Method relies on the initial values of the unknowns in two different cases and provides approximate solutions of the problem in the series form. To check the accuracy of the Rach Adomian Decomposition Method, We have compared the outcomes of this approach with those of the IM method. The RADM method is shown to give good results.

Keywords: Rach Adomian Decomposition Method, Iteration Method, Chemical Kinetics Systems, Non-linear Ordinary Differential Equations.

1. Introduction

Differential equations play a pivotal role in numerous disciplines of physical sciences, life sciences, mathematical sciences, engineering and technology¹⁻⁶. Many of the problems in differential equations are nonlinear, which are in the form of non-linear initial and boundary value problems. Discovering solutions for such non-linear problems is essential as well as stimulating. These may be exact analytical solutions or approximate numerical solutions. While the exact solutions are very difficult, in some cases, these equations might be overly complex for practical application, and at times, it may be impossible to find a solution. In this paper, a non-linear problem from the chemical sciences is considered. Such problems often involve nonlinear reactions with oscillatory influxes of reactants into a reaction medium. These phenomena of chemical kinetics typically manifest as a system of simultaneous non-linear ordinary differential equations (ODEs) in 3D. Oscillations and frequencies are pervasive in various scientific

domains, ranging from the rhythmic beating of the human heart, ecological systems like the Kolmogorov model etc. The systems of chemical kinetics that deviate significantly from equilibrium display a diverse array of phenomena, including chemical entropy. These systems can exhibit steady states. Sometimes these may result in chemical oscillations and in some cases, these may show chaotic dynamics as well⁷. The chemical kinetics system can be modeled as follows

$$(1) \quad \frac{dx_i}{dt}(t) = g_1(t, x_1(t), x_2(t), \dots, x_q(t)), x_i(t)_{t=0} = \beta_i, i = 1, 2, 3, \dots, q.$$

In this equation, β_i represents an identified constant vector, whereas $x_i(t)$ is the solution vector. In the paper⁸, the authors dealt with chemical applications employing a regular Homotopy Perturbation Method (HPM) and Variational Iteration Method (VIM). Matinfar *et al.*⁹ presented the approximate analytical solutions of the kinetics system using the analytic Homotopy Analysis Method (HAM).

In this paper, we have implemented the Rach Adomian Decomposition method (RADM) to solve the chemical kinetic system, which was first introduced by George Adomian, an American mathematician¹⁰, was the pioneer in developing the Adomian Decomposition Method (ADM). A lot of modifications have been done by various researchers for different purposes. The Adomian Decomposition Method (ADM) is a semi-analytical technique applicable for solving partial and ordinary differential equations of both linear and nonlinear orders. It is versatile enough to handle higher-order nonlinear differential equations and has found applications in various fields, such as fluid dynamics¹¹⁻¹³, as well as in numerical analysis¹⁴. This study emphasizes the significant role that ADM plays in addressing proposed chemical kinetics systems. In this work, the Rach Adomian Decomposition Method (RADM) has been employed to tackle a non-linear system of differential equations arising in chemical kinetics. A notable significance of RADM lies in the straightforward solution method, often allowing for accurate results within a minimal number of iterations.

The structure of this paper is outlined as follows: section 2 presents materials and methods for solving nonlinear chemical kinetic system, section 3 represents a Mathematical representation of systems governing chemical kinetics with two different cases, section 4 represents a basic definition of Rach Adomian Decomposition Method, section 5 is Results and Discussions of the Model of chemical kinetic system by Rach Adomian Decomposition Method, Section 6 provides a concise conclusion.

2. Materials and Methods

Understanding the pace of chemical processes is the focus of the physical science discipline known as chemical kinetics, also commonly referred to as reaction kinetics. Chemical kinetics processes can be studied by using different frequency computations to produce kinetic parameters^{15,16}. For the reaction to occur, the frequency of molecular collisions requires that the particles be oriented correctly and that the temperature be at the right level^{17,18}. Furthermore, the response rate can be increased by the impact of external vibrations at a frequency that corresponds to the intrinsic intermediate concentration and oscillations¹⁹. Different vibrations can affect how a chemical reaction proceeds, as shown by experimental studies of the kinetics of chemical reactions involving vibrationally stimulated molecules²⁰. Let us consider the following interaction expressions for the compounds $\mathcal{P}$, $\mathcal{Q}$ and $\mathcal{R}$ in a chemical kinetics model:



Let the concentrations of these substances $\mathcal{P}$, $\mathcal{Q}$ and $\mathcal{R}$ be denoted as x , y and z , respectively. Let equation (2) represent the reaction rate, signifying that the rate at which y goes up and x goes down, due to the reaction and it equals to αx . In another scenario, the rate of reaction is denoted as β in equation (3), and $\mathcal{R}$ acts as a catalyst when $\mathcal{P}$ is produced from $\mathcal{Q}$. This implies that x goes up while at the same time z goes down in this particular reaction. The resulting reaction rate equals to βyz . Finally, the reaction rate in the third equation is given by γy^2 because the construction of $\mathcal{R}$ from $\mathcal{Q}$ has a constant rate equal to γ .

3. The Model Of Chemical Kinetics Systems With Two Different Cases

To explain the chemical reactions that we just discussed above, the following example is taken from the chemistry problem^{21,22}

$$(5) \quad \frac{dx}{dt} = -\alpha x + \beta yz$$

$$(6) \quad \frac{dy}{dt} = \alpha x - \beta yz - \gamma y^2$$

$$(7) \quad \frac{dz}{dt} = \gamma y^2$$

with these initial conditions

Case I: $x(0) = 1, y(0) = 0, z(0) = 0$

Case II: $x(0) = 10, y(0) = 5, z(0) = 20$

and the parameters for the reaction rates are as follows:

$$\alpha = 0.1, \quad \beta = 0.02, \quad \gamma = 0.00$$

4. Rach Adomian Decomposition Method (ADM)

Adomian provided a comprehensive formula for solving all types of non-linear equations, yielding both analytic solutions and numerical approximations for both linear and nonlinear polynomials²³⁻²⁵. A lot of developments have been made in the original method by several authors for the calculation of Adomian polynomials. In 1990, Adomian and Rach presented a reliable development to this classical Adomian method which is slightly faster than the original polynomials.

Generally, in the Adomian decomposition method, the solution of a differential equation is expressed as a series, given by $u = \sum_{n=0}^{\infty} u_n$ and $f(u) = \sum_{n=0}^{\infty} A_n(u_0, u_1, \dots, u_n)$ where u_0 is a function that incorporates initial or boundary conditions. This gives the impression that solutions and solutions of function expand in the A_n polynomials. The formula of A_n polynomials can be expressed as $A_n = \frac{1}{n!} \left[\frac{d^n}{d\lambda^n} f(u(\lambda)) \right]_{\lambda=0}$ which is provided by Adomian, where 'n' is any positive integer that can be generated through the integer partition of 'n', which calculate the Adomian polynomials very fast and easily to obtain the analytical or approximate solutions which are defined as follows

For $n \geq 1, C_n^1 = u_n$ and for $2 \leq k \leq n, C_n^k = \frac{1}{n!} \sum_{j=0}^{n-k} (j+1) u_{j+1} C_{n-1-j}^{k-1}$

Then the formula of Adomian polynomials is shown as

$$A_0 = N(u_0), \text{ and } A_n = \sum_{k=1}^n N^k(u_0) C_n^k, \text{ for } n \geq 1.$$

This formula does not involve any differentiation operator, but requires only addition and multiplications for the coefficient C_n^k . This algorithm is highly suitable for solving both linear and nonlinear differential equations, irrespective of the type of initial or boundary conditions.

4.1. Solution of the Model of the chemical kinetic system by Rach Adomian Decomposition Method

Utilizing the differential operator L , defined as $L = \frac{d}{dt}(\cdot)$, and an inverse operator of L as L^{-1} , defined as $L^{-1} = \int_0^t (\cdot) dt$, As equations (5), (6), and (7) form a set of first-order ordinary differential equations with an initial value problem, they can be expressed as:

$$(8) \quad x(t) - x(0) = L^{-1}[-\alpha x] + L^{-1}[\beta yz]$$

$$(9) \quad y(t) - y(0) = L^{-1}[\alpha x] - L^{-1}[\beta yz] - L^{-1}[\gamma y^2]$$

$$(10) \quad z(t) - z(0) = L^{-1}[\gamma y^2]$$

The Adomian decomposition method allows the decomposition of x, y and z into infinite series components which is defined as

$$x(t) = \sum_{n=0}^{\infty} x_n, \quad y(t) = \sum_{n=0}^{\infty} y_n \quad \text{and} \quad z(t) = \sum_{n=0}^{\infty} z_n$$

The nonlinear terms in the provided model are yz and y^2 are presumed to take the following forms:

$$yz = \sum_{n=0}^{\infty} A_n \quad \text{and} \quad y^2 = \sum_{n=0}^{\infty} B_n$$

where A_n and B_n can be defined as $A_0 = N(u_0)$, and $A_n = \sum_{k=1}^n N^k(u_0) C_n^k$ for $n \geq 1$ and $B_0 = N(u_0)$, and $B_n = \sum_{k=1}^n N^k(u_0) C_n^k$ for $n \geq 1$.

For $n \geq 1$, $C_n^1 = u_n$ and for $2 \leq k \leq n$, $C_n^k = \frac{1}{n!} \sum_{j=0}^{n-k} (j+1) u_{j+1} C_{n-1-j}^{k-1}$.

By solving equations (8), (9) and (10) gives

$$(11) \quad \sum_{n=0}^{\infty} x_n = x(0) + -\alpha L^{-1} \sum_{n=0}^{\infty} x_n + \beta L^{-1} \sum_{n=0}^{\infty} A_n$$

$$(12) \quad \sum_{n=0}^{\infty} y_n = y(0) + \alpha L^{-1} \sum_{n=0}^{\infty} x_n - \beta L^{-1} \sum_{n=0}^{\infty} A_n - \gamma L^{-1} \sum_{n=0}^{\infty} B_n$$

$$(13) \quad \sum_{n=0}^{\infty} z_n = z(0) + \gamma L^{-1} \sum_{n=0}^{\infty} B_n$$

with the initial values, the solution of the system can be obtained, and the iterations are determined by the following recursive formulas as expressed:

$$(14) \quad \begin{aligned} x_0 &= x(0), \\ x_{n+1} &= -\alpha L^{-1} \sum_{n=0}^{\infty} x_n + \beta L^{-1} \sum_{n=0}^{\infty} A_n \end{aligned}$$

$$(15) \quad \begin{aligned} y_0 &= y(0), \\ y_{n+1} &= \alpha L^{-1} \sum_{n=0}^{\infty} x_n - \beta L^{-1} \sum_{n=0}^{\infty} A_n - \gamma L^{-1} \sum_{n=0}^{\infty} B_n \end{aligned}$$

and

$$(16) \quad \begin{aligned} z_0 &= z(0) \\ z_{n+1} &= \gamma L^{-1} \sum_{n=0}^{\infty} B_n \end{aligned}$$

The solutions are defined by X, Y and Z as

$$(17) \quad X = x_0 + x_1 + x_2 + x_3 + x_4 + x_5 + \dots \dots \dots$$

$$(18) \quad Y = y_0 + y_1 + y_2 + y_3 + y_4 + y_5 + \dots \dots \dots$$

$$(19) \quad Z = z_0 + z_1 + z_2 + z_3 + z_4 + z_5 + \dots \dots \dots$$

4.2. Numerical results

For case I: Given that initial conditions are $x(0) = 1$, $y(0) = 0$, $z(0) = 0$ and parameters values are $\alpha = 0.1$, $\beta = 0.02$, $\gamma = 0.009$, we obtained

$$x_1 = -0.1t, \quad y_1 = 0.1t, \quad z_1 = 0,$$

$$\begin{aligned}
x_2 &= 0.005t^2, & y_2 &= -0.005t^2, & z_2 &= 0 \\
x_3 &= -0.000166666667t^3, & y_3 &= 0.000136666667t^3 \\
z_3 &= 0.00003t^3 \\
x_4 &= 4.166666666668 \times 10^{-6}t^4, & y_4 &= -1.916666666668 \times 10^{-6}t^4 \\
z_4 &= -0.00000225t^4 \\
x_5 &= -7.133333333336 \times 10^{-8}t^5, & y_5 &= -2.286666666664 \times 10^{-8}t^5 \\
z_5 &= 9.4200000000001 \times 10^{-8}t^5 \\
&\cdot \\
&\cdot \\
&\cdot
\end{aligned}$$

and so forth. Following a similar approach, additional components can also be calculated. In this way, we get the approximate series solutions as follows:

$$\begin{aligned}
x(t) &= \sum_{n=0}^{\infty} x_n = 1 - 0.1t + 0.005t^2 - 0.000166666667t^3 \\
&\quad + 4.166666666668 \times 10^{-6}t^4 - 7.133333333336 \times 10^{-8}t^5 \dots \dots \dots \\
y(t) &= \sum_{n=0}^{\infty} y_n = 0.1t - 0.005t^2 + 0.000136666667t^3 \\
&\quad - 1.916666666668 \times 10^{-6}t^4 - 2.286666666664 \times 10^{-8}t^5 \dots \dots \dots \\
z(t) &= \sum_{n=0}^{\infty} z_n = 0.00003t^3 - 0.00000225t^4 \\
&\quad + 9.4200000000001 \times 10^{-8}t^5 \dots \dots \dots
\end{aligned}$$

For case II: where initial conditions are $x(0) = 10$, $y(0) = 5$, $z(0) = 20$, we obtained

$$\begin{aligned}
x_1 &= 1t \\
y_1 &= -1.225t \\
z_1 &= 0.225t \\
x_2 &= -0.28375t^2 \\
y_2 &= 0.33887500000t^2 \\
z_2 &= -0.055125t^2 \\
x_3 &= 0.050966666666t^3 \\
y_3 &= -0.065634791666666t^3 \\
z_3 &= 0.014668125t^3 \\
x_4 &= -0.0067520677083332t^4 \\
y_4 &= 0.01009689895833t^4 \\
z_4 &= -0.00334483125t^4 \\
x_5 &= 0.0006702295833330t^5 \\
y_5 &= -0.00134812847395833t^5 \\
z_5 &= 0.00067789889062499t^5 \\
&\cdot \\
&\cdot \\
&\cdot
\end{aligned}$$

and so forth. Following a similar approach, additional components can also be calculated. In this way, we get the approximate series solution as follows:

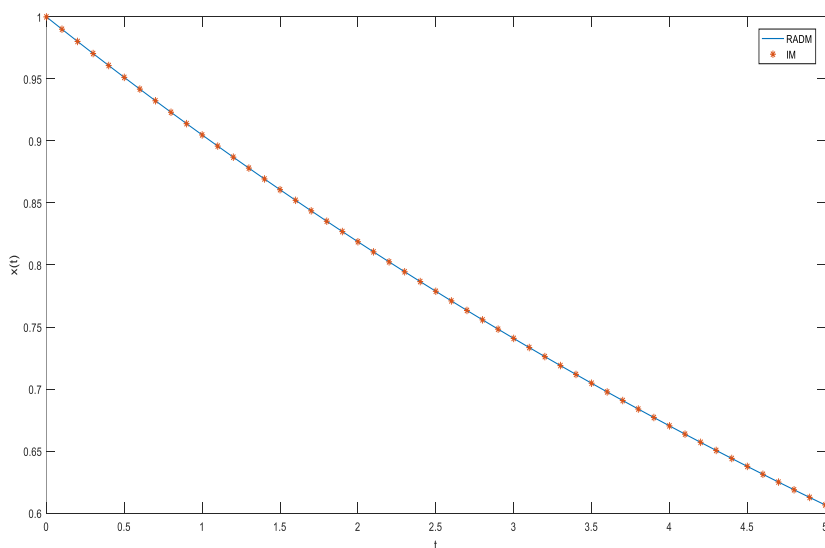
$$\begin{aligned}
 x(t) &= \sum_{n=0}^{\infty} x_n = 10 + t - 0.28375t^2 + 0.0509666666666t^3 \\
 &\quad - 0.0067520677083332t^4 + 0.0006702295833330t^5 - \dots \dots \dots \\
 y(t) &= \sum_{n=0}^{\infty} y_n = 5 - 1.225t + 0.33887500000t^2 - 0.0656347916666666t^3 \\
 &\quad + 0.01009689895833t^4 - 0.00134812847395833t^5 \dots \dots \dots \\
 z(t) &= \sum_{n=0}^{\infty} z_n = 20 + 0.225t - 0.055125t^2 + 0.014668125t^3 \\
 &\quad - 0.00334483125t^4 + 0.00067789889062499t^5 - \dots \dots \dots
 \end{aligned}$$

5. Results and Discussion

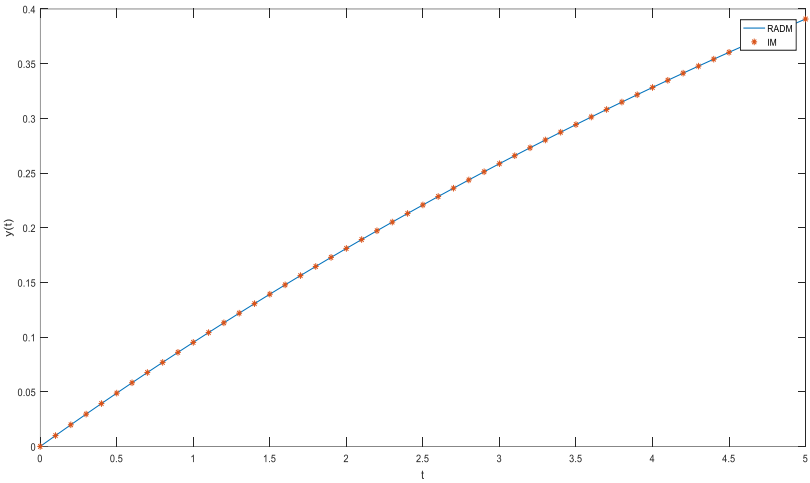
In general, no exact solutions are available for nonlinear chemical kinetics systems of ordinary differential equations so we have compared our results with the Iteration method. Furthermore, utilizing the Rach Adomian Decomposition Method (RADM), we have obtained highly accurate series solutions with just five iterations in all instances. In the following Figures and a comparison graphs between the Iterative Method and Adomian Decomposition Method are given in the next section.

Figures for case I and case II

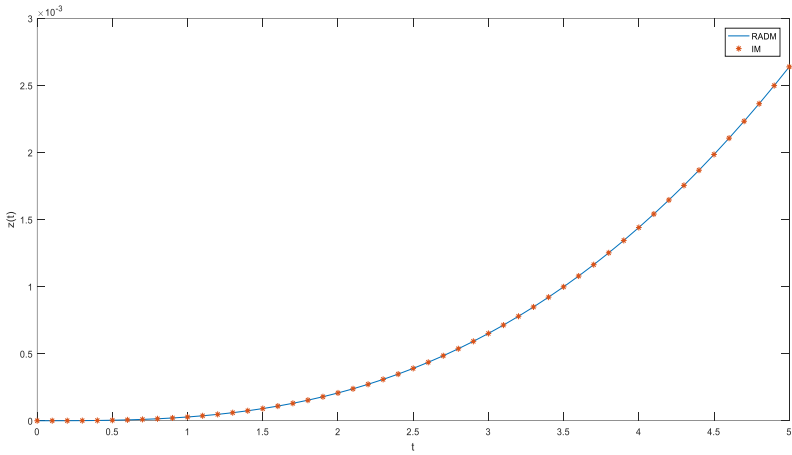
For case I



(a)



(b)

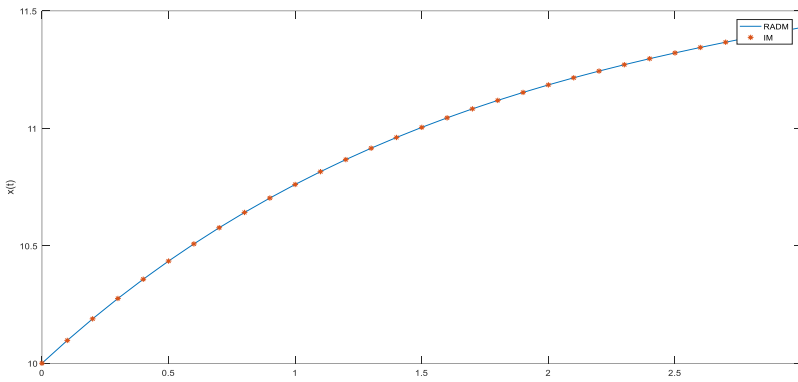


(c)

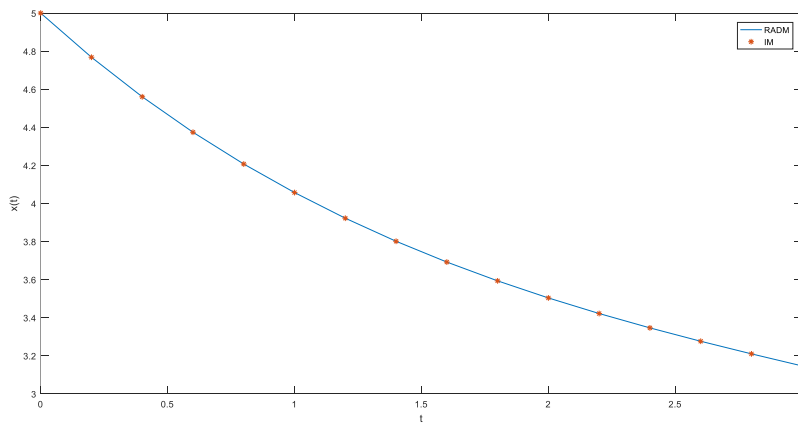
Figure 1: Comparative graphs for x, y and z depicting RADM (solid blue line) and IM (dotted red dashes) for Case I

Numerical approximations have been carried out using the initial conditions provided in equation (17) and with the parameters of reaction rate $\alpha = 0.1$, $\beta = 0.02$, $\gamma = 0.009$. It has been observed that solutions given by AL-Jawary *et. al.*²² remain valid during a limited time domain $t = 0$ to 0.1 only. In contrast, Figure 1 clearly demonstrates that our proposed solutions using RADM consistently yield more accurate results, even in the extended time domain $t = 0$ to 5 .

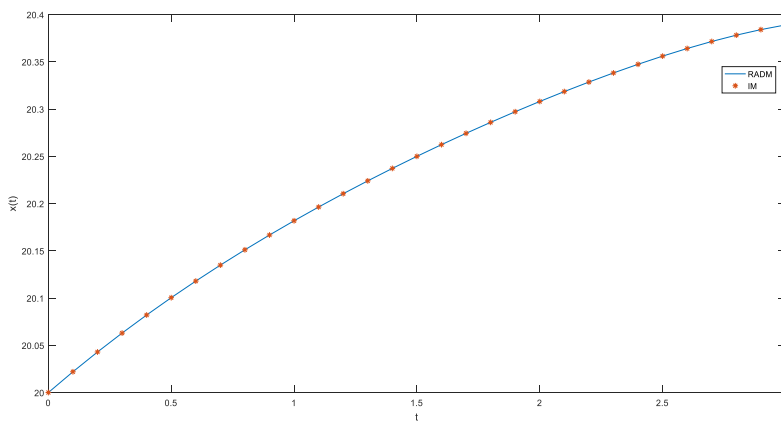
For case II



(a)



(b)



(c)

Figure 2. Comparative graphs for x , y and z depicting RADM (solid blue line) and IM (dotted red dashes) for Case II

Analogous to the previously mentioned instance, we have contrasted the numerical outcomes of RADM with IM in a limited time frame = 0 to 0.1 . The computations were performed using alternative initial conditions specified in equation (18) and parameters reaction rate $\alpha = 0.1$, $\beta = 0.02$, $\gamma = 0.009$.

Many non-linear systems can be solved with the help of various numerical methods. However, analytical series solutions²⁶ cannot find with the help of some numerical methods such as RK4. But, explicit solutions and numeric solutions can be obtained through analytical methods such as RADM. The initial iteration steps of RADM closely resemble those of the Homotopy Perturbation Method (HPM)¹⁹ and the Variational Iteration Method (VIM)²⁷.

6. Conclusion

In this study, the modified Adomian Decomposition Method is employed, *i.e.* RADM for solving nonlinear Chemical Kinetic systems with the initial conditions of first-order nonlinear ordinary differential equations considered in two distinct cases. The Rach Adomian Decomposition method has been introduced. In each case, The numerical solutions obtained through the Modified Adomian Decomposition Method are compared with those obtained through the iterative method. The RADM made a perfect agreement with the semi-analytical method, *i.e.* IM. Therefore, it is resolved that RADM is a superior instrument for getting solutions of many types of system of non-linear differential equations.

References

1. MSH Chowdhury, I Hashim and H-R. Roslan; Simulation of the predator-prey problem by the homotopy-perturbation method revise, *Topol Methods Nonlinear Anal J Juliusz Schauder Cent*, 31 (2008), 263-270.
2. M A Hosen and MSH Chowdhury, A new analytical technique based on harmonic balance method to determine approximate periods for Duffing-harmonic oscillator, *Alexandria Eng J* , 54 (2015), 233-239.
3. MSH Chowdhury and I Hashim; Application of homotopy-perturbation method to Klein-Gordon and sine-Gordon equations, *Chaos Solitons Fractal*, 39 (2009), 1928-1935.
4. MSH Chowdhury and I Hashim; Solutions of time-dependent Emden-Fowler type equations by homotopy-perturbation method, *Phys Lett Sect A Gen At Solid State Phys*, 368 (2007), 305-313.

5. M S H Chowdhury, I Hashim and O Abdulaziz; Application of homotopy-perturbation method to nonlinear population dynamics models, *Phys Lett Sect A Gen At Solid State Phys*, 368 (2007), 251-258.
6. I Hashim, MSH Chowdhury and S Mawa; On multistage homotopy-perturbation method applied to nonlinear biochemical reaction model, *Chaos Solitons Fractal*, 36 (2008), 823-827.
7. P L Gentili and JC Micheau; Light and chemical oscillations: review and perspectives, *J Photochem Photobiol C Photochem Rev*, 43 (2020), 100321.
8. D D Ganji, M Nourollahi and E Mohseni; Application of He's methods to nonlinear chemistry problems, *Comput Math Appl*, 54 (2007), 1122-1132.
9. M Matinfar, M Saeidy, B Gharahsuflu; Solutions of nonlinear chemistry problems by homotopy analysis, *Comput Math Model*, 25 (2014), 103-114.
10. G. Nwawu, P. Mafuta, J. Mushanyu; The Adomian Decomposition Method for Numerical Solution of First Order Differential Equations, *J. Math. Comput. Sci.*, 6 (2016), 307-314.
11. M. Jiya, J. Oyubu; Adomian Decomposition Method for the Solution of Boundary Layer Convective Heat Transfer with Low Pressure Gradient over a Flat, *IOSR J. Math.*, 4 (2012), 34-42. doi: 10.9790/5728-0413442
12. A. Adeniyani, A. I. Abioye; Mixed Convection Radiating Flow and Heat Transfer in a Vertical Channel Partially Filled with a Darcy-Forchheimer Porous Substrate, *Gen. Math. Notes*, 32 (2016), 80-104.
13. H. Heidarzadeh, J. M. Mashinchi, R. Asghari; Application of Adomian Decomposition Method to Nonlinear Heat Transfer Equation, *The J. Math. Comp. Sci.*, 4 (2012), 436-447.
14. M Cakir, D Arslan; The Adomian Decomposition Method and the Differential Transform Method for Numerical Solution of Multi-Pantograph Delay Differential Equations, *Appl. Math.*, 6 (2015), 1332-1343. doi:10.4236/am.2015.68126.
15. A Ghysels, T Verstraelen, K Hemelsoet; A versatile package for vibrational analysis and chemical kinetics, *J Chem Inf Model*, 50 (2010), 1736-1750.
16. G Feher and M Weissman; Fluctuation spectroscopy, Determination of chemical reaction kinetics from the frequency spectrum of fluctuations, *Proc Natl Acad Sci USA* 70 (1973), 870-875.
17. K J Laidler; The development of the Arrhenius equation, *J Chem Educ*, 61 (1984), 494-498.
18. P Ptacek, T Opravil, F Soukal; *A brief introduction to the history of chemical kinetics*, In: *Introducing the Effective Mass of Activated Complex and the Discussion on the Wave Function of this Instanton*, IntechOpen Limited, 2018.
19. L P Smirnov, TP Kulagina and ZS Andrianova; Influence of low-frequency vibrations on the chemical reaction rate in the liquid phase for reagent association, *Russ Chem Bull*, 66 (2017), 30-33.

20. FF Crim; Chemical dynamics of vibrationally excited molecules: controlling reactions in gases and on surfaces, *Proc Natl Acad Sci USA*, 105 (2008), 12654-12661.
21. M M Khader; On the numerical solutions for chemical kinetics system using Picard–Pade technique, *J King Saud Univ - Eng Sci*, 25 (2013), 97-103.
22. MA Al-Jawary and RK Raham; A semi-analytical iterative technique for solving chemistry problems, *J King Saud Univ – Sci*, 29 (2017), 320-332.
23. G Adomian, R Rach; Generalization of Adomian polynomials to functions of several variables, *Computer Math. Applic.*, 24(5/6) (1992), 11-24.
24. G Adomian; A review of the decomposition method in applied mathematics, *J. Math. Anal. Appl.*, 135 (1988), 501-544.
25. G Adomian; *Nonlinear stochastic operator equations*, Academic Press, New York, 1986.
26. AA Hemeda; New iterative method: an application for solving fractional physical differential equations, *Abstr Appl Anal*, 1 (2013), Article ID 617010, 9 pages, <http://dx.doi.org/10.1155/2013/617010>.
27. J H He; Variational iteration method – some recent results and new interpretations, *J Comput Appl Math*, 207 (2007), 3-17.