CAND

Computational Algorithms and Numerical Dimensions

www.journal-cand.com

Com. Alg. Num. Dim Vol. 1, No. 3 (2022) 98–103.

Paper Type: Original Article

Analytical Approximate Solution of Chemical Kinetics Problems

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Citation:

Günerhan, H. (2022). Analytical approximate solution of chemical kinetics problems. *Computational algorithms and numerical dimensions, 1*(3), 98-103.

Received: 23/08/2022 Reviewed: 20/09/2022 Revised: 23/10/2022 Accept: 11/11/2022

Abstract

In this article, the chemical kinetics problem is presented. The Differential Transformation Method (DTM) is presented to find an approximate analytical solution to the chemical kinetics problems. Proposed problem is system of nonlinear ordinary differential equations. We show converges analysis of the differential transform method. DTM applied to two examples. The method shows the form of fast converging series and the results prove the applicability of the proposed method, which gives accurate results.

Keywords: Chemical kinetic problems, Differential transform method, Power series, Approximate analytical solution.

1 | Introduction

In this paper we are concerned chemical kinetics problems system;

$$\frac{dx_1}{dt} = -a_1x_1 + a_2x_2x_3,$$
$$\frac{dx_2}{dt} = a_1x_1 - a_2x_2x_3 - a_3{x_2}^2, \quad (1)$$
$$\frac{dx_3}{dt} = a_3{x_2}^2.$$

With the initial conditions;

$$x_1\ 0) = 1, x_2\ 0) = 0, x_3\ 0) = 0. \quad (2)$$

Where a_1, a_2 and a_3 are the reaction rates. In chemistry the chemical kinetics system is well described by nonlinear system of ordinary differential equations. Robertson [4] introduced the system in 1966, indicating the mathematical model of a chemical kinetic problem [1], [2].

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https://doi.org/10.22105/cand.2022.155255

In recent years, numerous works have been focusing on the development of more advanced and efficient methods for the Homotopy Perturbation Method (HPM) and the Variation Iteration Method (VIM) [2], the picard-pade technique [3], the homotopy analysis method [3] and the Adomian's decomposition method [5] and iterative method [6]. The Differential Transformation Method (DTM) was first created by Zhou [7] to obtain approximate-analytical solutions to ordinary differential equations using Taylor series formulation. The differential transform method obtains an analytical solution in the form of a polynomial. It is different from the traditional high order Taylor's series method, which requires symbolic competition of the necessary derivatives of the data functions. The results of applying DTM to the chemical kinetics problems will be presented.

2 | Differential Transform Method

Differential transform of function $y(x)$ is defined as follows:

$$Y\ k) = \frac{1}{k!}\left[\frac{d^k y(x)}{dx^k}\right]_{x=0}. \tag{3}$$

In *Eq. (3)*, $y\ x)$is the original function and $Y(k)$ is the transformed function, which is called the T-function. Differential inverse transform of $Y(k)$ is defined as

$$y\ x) = \sum_{k=0}^{\infty} x^k Y\ k). \tag{4}$$

From *Eq. (3)* and *(4)*, we obtain

$$y\ x) = \sum_{k=0}^{\infty} \frac{x^k}{k!}\left[\frac{d^k y(x)}{dx^k}\right]_{x=0}. \tag{5}$$

Eq. (5) implies that the concept of differential transform is derived from Taylor series expansion, but the method does not evaluate the derivatives symbolically.

However, relative derivatives are calculated by an iterative way which are described by the transformed equations of the original functions. In this study we use the lower case letter to represent the original function and upper case letter represent the transformed function.

From the definitions of *Eqs. (2)* and *(4),* it is easily proven that the transformed functions comply with the basic mathematics operations shown in *Table 1*.

In actual applications, the function $y(x)$ is expressed by a finite series and *Eq. (4)* can be written as:

$$y\ x) = \sum_{k=0}^{m} x^k Y\ k). \tag{6}$$

Eq. (5) implies that $\sum_{k=m+1}^{\infty} x^k Y\ k)$, is negligibly small. In fact, m is decided by the convergence of natural frequency in this study.

Table 1. The fundamental operations of DTM.

Original Function	Transformed Function
$y(x) = u(x) \pm v(x)$	$Y(k) = U(k) \pm V(K)$
$y(x) = cw(x)$	$Y(k) = cW(k)$
$y(x) = dw/dx$	$Y(k) = (K+1)W(k+1)$
$y(x) = d^j w/dx^j$	$Y(k) = (K+1)(K+2) \ldots (K+j)W(k+j)$
$y(x) = u(x)v(x)$	$Y(k) = \sum_{r=0}^{k} U(r)V(K-r)$

Theorem 1. If $y\ x) = exp(x)$ then $\ k) = \frac{1}{k!}$.

Proof. By using *Eq. (3)*, we have

$$W\ k) = \frac{1}{k!}\frac{\partial(e^x)}{\partial x^k}\bigg|_{t=0} = \frac{1}{k!}e^x\bigg|_{t=0} = \frac{1}{k!}.$$

Theorem 2. If $y\ x) = \frac{\partial^m u(x)}{\partial x^m}$ then $Y\ k) = \frac{k+m)!}{k!}U\ k+m)$.

Proof. By using *Eq. (3)*, we have;

$$Y\ k) = \frac{1}{k!}\frac{\partial^k}{\partial x^k}\frac{\partial^m u\ x)}{\partial x^m}\bigg|_{t=0} = \frac{1}{k!}\frac{\partial^{m+k}u\ x)}{\partial x^{m+k}}\bigg|_{t=0} = \frac{k+m)!}{k!}U\ k+m).$$

Theorem 3. If $y\ x) = x^m$ then $k) = \delta\ k-m) = \begin{cases}1 & k=m\\ 0 & k\neq m\end{cases}$.

Proof. By using *Eq. (3)*, we have;

$$W\ k) = \frac{1}{k!}\frac{\partial\ x^m)}{\partial x^k}\bigg|_{t=0} = \begin{cases}\frac{1}{k!}\frac{\partial^k(x^k)}{\partial x^k} = \frac{k!}{k!} = 1, & k=m\\ \frac{1}{k!}\frac{\partial^k\ x^m)}{\partial x^k} = 0\,, & k\neq m\end{cases}.$$

Theorem 4. If $w\ x) = \sin(wx+\alpha)$ then $W\ k) = \frac{w^k}{k!}\sin(\frac{k\pi}{2}+\alpha)$.

Proof. By using *Eq. (3)*, we have;

$$k=1\quad W\ 1) = \frac{1}{1!}\frac{\partial\sin\ wx+\alpha)}{\partial x}\bigg|_{x=0} = \frac{1}{1!}w\cos\ wx+\alpha)\bigg|_{x=0} = \frac{1}{1!}w\sin\left(\left(\frac{\pi}{2}+\alpha\right)+wx\right)\bigg|_{x=0}$$

$$= \frac{1}{1!}w\sin\left(\frac{\pi}{2}+\alpha\right),$$

$$k=2\quad W\ 2) = \frac{1}{2!}\frac{\partial^2\sin\ wx+\alpha)}{\partial x^2}\bigg|_{x=0} = \frac{1}{2!}w^2\cos\left(wx+\frac{\pi}{2}+\alpha\right)\bigg|_{x=0}$$

$$= \frac{1}{2!}w^2\sin\left(\frac{\pi}{2}+\left(\frac{\pi}{2}+\alpha\right)+wx\right)\bigg|_{x=0} = \frac{1}{2!}w^2\sin\left(\frac{2\pi}{2}+\alpha+wx\right)\bigg|_{x=0} = \frac{1}{2!}w^2\sin\left(\frac{2\pi}{2}+\alpha\right).$$

In the general form we have;

$$k=n\quad W\ n) = \frac{1}{k!}\frac{\partial^n\sin\ wx+\alpha)}{\partial x^n}\bigg|_{x=0} = \frac{1}{n!}w^n\sin(wx+\frac{n\pi}{2}+\alpha)\bigg|_{x=0} = \frac{1}{n!}w^n\sin\left(\frac{n\pi}{2}+\alpha\right).$$

Theorem 5. If $w\ x) = \cos(wx+\alpha)$ then $W\ k) = \frac{w^k}{k!}cos(\frac{k\pi}{2}+\alpha)$.

Proof. By using *Eq. (3)*, we have;

$$k=1\quad W\ 1) = \frac{1}{1!}\frac{\partial\cos\ wx+\alpha)}{\partial x}\bigg|_{x=0} = \frac{-1}{1!}w\sin\ wx+\alpha)\bigg|_{x=0}$$

$$= \frac{1}{1!}w\cos(\left(\frac{\pi}{2}+\alpha\right)+wx)\bigg|_{x=0} = \frac{1}{1!}w\cos\left(\frac{\pi}{2}+\alpha\right),$$

$$k=2\quad W\ 2) = \frac{1}{2!}\frac{\partial^2\cos\ wx+\alpha)}{\partial x^2}\bigg|_{x=0} = \frac{-1}{2!}w^2\sin\left(wx+\frac{\pi}{2}+\alpha\right)\bigg|_{x=0}$$

$$= \frac{1}{2!}w^2\cos\left(\frac{\pi}{2}+\left(\frac{\pi}{2}+\alpha\right)+wx\right)\bigg|_{x=0} = \frac{1}{2!}w^2\cos\left(\frac{2\pi}{2}+\alpha+wx\right)\bigg|_{x=0} = \frac{1}{2!}w^2\cos\left(\frac{2\pi}{2}+\alpha\right).$$

In the general form we have;

$$k=n\quad W\ n) = \frac{1}{k!}\frac{\partial^n\cos\ wx+\alpha)}{\partial x^n}\bigg|_{x=0} = \frac{1}{n!}w^n\cos(wx+\frac{n\pi}{2}+\alpha)\bigg|_{x=0} = \frac{1}{n!}w^n\cos\left(\frac{n\pi}{2}+\alpha\right).$$

In this part, we will show converges of the differential transform method to the exact solution by proof of some theorems [8].

Theorem 6. Consider the first order ordinary differential equation in here m, n are constants;

$$m\,\frac{dw(x)}{dx} + nw\ x) = 0, w\ 0) = \gamma. \tag{7}$$

The differential transform method converges to the exact solution.

Proof. The general solution of differential equation is as $w\ x) = \beta e^{-nx/m}$.

Now by taking the differential transform of *Eq. (7)*, we have;

$$m\,W[K+1] + nW[K] = 0,\ \ W[0] = \beta.$$

We have $W[K+1] = \frac{-nW[K]}{m}$. By solve this recurrence relation, we get $W[K] = \frac{1}{k!}\left(\frac{-n}{m}\right)^{k}\beta$.

By using *Eq. (8)*, the solution obtained by DTM is as follows:

$$w\ x) = \beta\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{-nx}{m}\right)^{k} = \beta e^{-\frac{nx}{m}}. \tag{8}$$

Theorem 7. Consider the homogeneous ordinary differential equation of order n, where $v_i, i = 1,2,\dots,n$ are variables;

$$v_0\ x)w + \sum_{r=1}^{n} v_r\ x)\frac{d^r w}{dx^r} = 0. \tag{9}$$

With initial conditions

$$w\ x) = \beta_0,\ \left.\frac{d^i w}{dx^i}\right|_{x=0} = \beta_i, i = 1,2,\dots,n-1\ . \tag{10}$$

The differential transform method converges to the exact solution.

Proof. By using with both *Table 1* and the *Eq. (9)*, we have;

$$\sum_{m=0}^{k}\left(V_0[k]W[k-m] + \sum_{r=1}^{n}\left[V_r[k]\left[\prod_{j=1}^{r} k-m+j)\right]W[k-m+r]\right]\right) = 0.$$

From the initial conditions, we have;

$$W[0] = \beta_0,\ \ W[i] = \frac{\beta_i}{i!}, i = 1,2,\dots,n-1.$$

By substituting the differential transforms, we have;

$$w\ x) = \sum_{k=0}^{\infty} W[k]x^k,\ \ v_r\ x) = \sum_{k=0}^{\infty} A_r[k]x^k.$$

Substituting the above formulas in *Eq. (9)*, we get;

$$0 = \sum_{k=0}^{\infty} A_0[k]x^k \sum_{k=0}^{\infty} W[k]x^k + \sum_{r=1}^{n}\left(\sum_{k=0}^{\infty} A_r[k]x^k . \left(\frac{d^r}{dx^r}\sum_{k=0}^{\infty} W[k]x^k\right)\right)$$
$$= \sum_{k=0}^{\infty}\sum_{m=0}^{\infty} A_0[m]\,W[k-m]x^k \sum_{r=1}^{n}\left(\sum_{k=0}^{\infty} A_r[k]x^k.\ \sum_{m=0}^{\infty} W[m+r])\left(\prod_{j=0}^{r-1} m + r - j)\right)x^m\right) = \sum_{k=0}^{\infty}\sum_{m=0}^{k}\left(A_0[m]W[k-m] + \sum_{r=1}^{n} A_r[m]W[k-m+r]\left(\prod_{j=1}^{r} k - m + j)\right)x^k.\right.$$

We comparing coefficients and get;

$$\sum_{m=0}^{k} A_0[m]W[k-m] + \sum_{r=1}^{n} A_r[m]W[k-m+r]\left(\prod_{j=1}^{r} k-m+j\right) = 0\ .$$

3 | Numerical Example

Example 1. We consider the system of chemical kinetics;

$$\frac{dx_1}{dt} = -a_1x_1 + a_2x_2x_3,$$
$$\frac{dx_2}{dt} = a_3x_1 - a_4x_2x_3 - a_5{x_2}^2, \tag{11}$$
$$\frac{dx_3}{dt} = a_6{x_2}^2.$$

With the initial conditions

$$x_1\ 0) = 1, x_2\ 0) = 0,\ \ x_3\ 0) = 0. \tag{12}$$

When taking the one dimensional differential transform of *Eq. (11)*, we can obtain:

$$
\begin{aligned}
&X_1\ n+1) = \frac{1}{(n+1)}[-a_1X_1\ n) + a_2 \textstyle\sum_{r=0}^{n} X_2\ r)X_3\ n-r)],\\
&X_2\ n+1) = \frac{1}{(n+1)}[a_3X_1\ n) - a_4 \textstyle\sum_{r=0}^{n} X_2\ r)X_3\ n-r) - a_5 \textstyle\sum_{r=0}^{n} X_2\ r)X_2\ n-r)],\\
&X_3\ n+1) = \frac{1}{(n+1)}[a_6 \textstyle\sum_{r=0}^{n} X_2\ r)X_2\ n-r)],
\end{aligned} \tag{13}
$$

The initial conditions can be transformed at $x_0 = 0$, as;

$$X_1\ 0) = 1\ , X_2\ 0) = 0\ ,\ X_3\ 0) = 0. \tag{14}$$

For $n = 0,1,2,\ldots,$ $X_1(n)$, $X_2(n)$, $X_3(n)$, coefficients can be calculated from *Eqs. (13)* and *(14)*;

$$
\begin{aligned}
&X_1\ 1) = -a_1,\ X_2\ 1) = a_3,\ X_3\ 1) = 0,\ X_1\ 2) = \frac{a_1{}^2}{2},\\
&X_2\ 2) = \frac{-a_3a_1}{2}, X_3\ 2) = 0,\ X_1\ 3) = \frac{-a_1{}^3}{6},\\
&X_2\ 3) = \frac{1}{3}\left(\frac{a_3\ a_1)^2}{2} - a_5\ a_3)^2\right),\ X_3\ 3) = \frac{a_6\ a_3)^2}{3}, \ldots .
\end{aligned} \tag{15}
$$

By using the inverse transformation rule for one dimensional in *Eq. (6)*, the following solution can be obtained:

$$
\begin{aligned}
&X_1\ t) = 1 - a_1t + \frac{a_1{}^2}{2}t^2 - \frac{a_1{}^3}{6}t^3 + \cdots,\\
&X_2\ t) = a_3t - \frac{a_3a_1}{2}t^2 + \frac{1}{3}\left(\frac{a_3\ a_1)^2}{2} - a_5\ a_3)^2\right)t^3 + \cdots,\\
&X_3\ t) = \frac{a_6\ a_3)^2}{3}t^3 + \cdots .
\end{aligned} \tag{16}
$$

Example 2. We consider the system of chemical kinetics;

$$
\begin{aligned}
&\frac{dx_1}{dt} = -x_1,\\
&\frac{dx_2}{dt} = x_1 - x_2{}^2,\\
&\frac{dx_3}{dt} = x_2{}^2.
\end{aligned} \tag{17}
$$

Subject to the initial conditions;

$$x_1\ 0) = 1, x_2\ 0) = 0, x_3\ 0) = 0. \tag{18}$$

When taking the one dimensional differential transform of *Eqs. (17)* and *(18)*, we can obtain:

$$
\begin{aligned}
&X_1\ n+1) = \frac{1}{(n+1)}[-X_1\ n)],\\
&X_2\ n+1) = \frac{1}{(n+1)}[X_1\ n) - \textstyle\sum_{r=0}^{n} X_2\ r)X_2\ n-r)],\\
&X_3\ n+1) = \frac{1}{(n+1)}\left[\sum_{r=0}^{n} X_2\ r)X_2\ n-r)\right].
\end{aligned} \tag{19}
$$

And

$$X_1\ 0) = 1\ , X_2\ 0) = 0\ , X_3\ 0) = 0. \tag{20}$$

For $n = 0,1,2,\ldots,$ $X_1(n)$, $X_2(n)$, $X_3(n)$, coefficients can be calculated from *Eqs. (19)* and *(20)*.

$$
\begin{aligned}
&x_1\ 1) = -1, x_2\ 1) = 1, x_3\ 1) = 0,\\
&x_1\ 2) = \frac{1}{2}, x_2\ 2) = \frac{-1}{2}, x_3\ 2) = 0,\\
&x_1\ 3) = \frac{-1}{6}, x_2\ 3) = \frac{-1}{6}, x_3\ 3) = \frac{1}{3}.
\end{aligned} \tag{21}
$$

By using the inverse transformation rule for one dimensional in *Eq. (6)*, the following solution can be obtained:

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$$X_1\ t) = 1 - t + \frac{t^2}{2} - \frac{t^3}{6} + \frac{t^4}{24} - \cdots,$$
$$X_2\ t) = t - \frac{t^2}{2} + \frac{t^3}{6} + \frac{5t^4}{24} \ldots, \tag{22}$$
$$X_3\ t) = \frac{t^3}{3} - \frac{t^4}{4} + \cdots.$$

4 | Conclusion

In this study, the differential transform method is successfully expanded for the solution of chemical kinetics problems. Since the DTM gives rapidly converging series solutions, the differential transform method is more effective than other methods. Finally, all results prove the validity and efficiency of these methods in solving nonlinear differential equations.

References

[1] Aminikhah, H. (2011). An analytical approximation to the solution of chemical kinetics system. *Journal of King Saud university-science*, *23*(2), 167-170.

[2] Ganji, D. D., Nourollahi, M., & Mohseni, E. (2007). Application of He's methods to nonlinear chemistry problems. *Computers & mathematics with applications*, *54*(7-8), 1122-1132.

[3] Khader, M. M. (2013). On the numerical solutions for chemical kinetics system using Picard–Padé technique. *Journal of King Saud university-engineering sciences*, *25*(2), 97-103.

[4] Robertson, H. H. (1966). The solution of a set of reaction rate equations. *Numerical analysis: an introduction*, *178182*.

[5] Eckes, T., & Trautner, H. M. (Eds.). (2000). *The developmental social psychology of gender*. Lawrence Erlbaum Associates Publishers.

[6] AL-Jawary, M., & Raham, R. (2016). Numerical solution for chemical kinetics system by using efficient iterative method. *International journal of advanced scientific and technical research*, *1*(6), 367-375.

[7] Zhou, J. K. (2000). *Differential transform and its applications for electrical circuits*. Huazhong University Press.

[8] Oke, A. S. (2017). Convergence of differential transform method for ordinary differential equations. *Journal of advances in mathematics and computer science*, *24*(6), 1-17.