Differentıal Transform Method for Solvıng a Boundary Value Problem Arısıng in Chemıcal Reactor Theory

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Abstract

In this study, we deal with the numerical solution of the mathematical model for an adiabatic tubular chemical reactor which processes an irreversible exothermic chemical reaction. For steady state solutions, the model can be reduced to the following nonlinear ordinary differential equation [1]:

$$u'' - \lambda u' + \lambda\mu(\beta - u)\exp(u) = 0, \tag{1}$$

where λ, μ and β are Péclet number, Damköhler number and adiabatic temperature rise, respectively.

Boundary conditions of Eq. (1) are

$$u'(0) = \lambda u(0), u'(1) = 0. \tag{2}$$

Differential transform method [2] is used to solve the problem (1)-(2) for some values of the considered parameters. Residual error computation is adopted to confirm the accuracy of the results. In addition, the obtained results are compared with those obtained by other existing numerical approach [3].

1. Introduction

In chemical engineering, chemical reactors are vessels designed to contain chemical reactions. These reactors are of importance because of their several industrial applications. Some areas of usage of tubular reactors are Algae production, biological treatment and gasoline production. In this study, an adiabatic tubular chemical reactor which processes an irreversible exothermic chemical reaction will be discussed. In particular, we obtain a positive solution $u(x)$, namely the solution $u(x)$ of Eq.(1), to the system represents the steady state temperature of the reaction.

Existence of solution to the problem (1)-(2) has been studied in [4] and [5]. Existence of multiple solutions was proved in [1]. Some numerical methods were applied to tackle the problem under investigation. For example, in [6], the Green's function is first utilized to convert the problem into Hammerstein integral equation. And then, the resulting equation was solved via Adomian's decomposition method. In [7], the method of Chebyshev finite difference was used to handle the problem. The authors of [3] approached the problem using a strategy which is based on embedding Green's function into Krasnoselskii–Mann's fixed point iteration scheme.

In this paper, we apply differential transform method (in short, DTM) as an alternative to existing methods to solve the problem (1)-(2) for some values of the considered parameters. The concept of differential transform method was first introduced in [8], which is solved linear and nonlinear initial value problems in electric circuit analysis. This method is useful to obtain the exact and approximate solutions of linear and nonlinear differential equations and does not require linearization or discretization.

2. The method of solution and the solution to the problem (1)-(2)

In this section, the fundamental idea of one dimensional differential transform method is concisely introduced [2].

2.1. One dimensional differential transform method

We assume that $u(x)$ is an analytic function in domain T and x_0 is any point in T. Then the function $u(x)$ can be expanded about x_0 using the Taylor expansion for every point x in T as follows:

$$u(x) = \sum_{k=0}^{\infty} \frac{1}{k!} \left[\frac{d^k u(x)}{dx^k}\right]_{x=x_0} (x - x_0). \tag{3}$$

The differential transformation of the function $u(x)$ is stated as:

$$U(k) = \frac{1}{k!} \left[\frac{d^k u(x)}{dx^k}\right]_{x=x_0}. \tag{4}$$

Here, $u(x)$ is the original function and $U(k)$ is the transformed function, respectively. Based on Eqs.(3) and (4), we are able to establish the correlation between $u(x)$ and $U(k)$:

$$u(x) = \sum_{k=0}^{\infty} U(k)(x - x_0)^k. \tag{5}$$

In real applications, function $u(x)$ is expressed by a finite series and Eq.(5) can be written as

$$u(x) = \sum_{k=0}^{N} U(k)(x - x_0)^k. \tag{6}$$

It is obvious that the differential transform method is build upon on the basis of Taylor series expansion. Hence the corresponding derivatives can be obtained by way of a recurrence relation that is described by the transformed equations of the original functions. In practical applications, the fucntion $u(x)$ is usually truncated at a certain order N and the residual error

$$u_r(x) = \sum_{k=N+1}^{\infty} U(k)(x - x_0)^k.$$

is negligible small. Usually, the value of N is such chosen that the error is less than a prescribed value. Some fundamentally mathematical operations that are used in the transformation of the differential equations are listed in Table 1.

Table 1. The fundamental operations of one dimensional differential transform method.

Original function	Transformed function
$f(x) = g(x) \pm h(x)$	$F(k) = G(k) \pm H(k)$
$f(x) = cg(x)$	$F(k) = cG(k)$
$f(x) = g(x)h(x)$	$F(k) = \sum_{l=0}^{k} G(l)H(k-l)$
$f(x) = \frac{d^m g(x)}{dx^m}$	$F(k) = \frac{(k+m)!}{k!} G(k+m)$

From the definitions of equations (4) and (5), it is easily proven that the transformed functions comply with the fundamental operations shown in Table 1. Now we prove some theorems given in Table I, which are essential to solving the problem (1)-(2).

Theorem I

If $f(x) = g(x)h(x)$, then $F(k) = \sum_{l=0}^{k} G(l)H(k-l)$.

Proof.

Starting with the k-th order derivative of the product of two functions like

$$\frac{d^k}{dx^k}[g(x)h(x)] = \sum_{i=0}^{k} \binom{k}{i} \frac{d^i}{dx^i}[h(x)] \frac{d^{k-i}}{dx^{k-i}}[g(x)]$$

$$= h(x) \frac{d^k}{dx^k}[g(x)] + \binom{k}{1} \frac{d}{dx}[h(x)] \frac{d^{k-1}}{dx^{k-1}}[g(x)] + \binom{k}{2} \frac{d^2}{dx^2}[h(x)] \frac{d^{k-2}}{dx^{k-2}}[g(x)]$$

$$+ \cdots + \binom{k}{k-1} \frac{d^{k-1}}{dx^{k-1}}[h(x)] \frac{d}{dx}[g(x)] + \left(\frac{d^k}{dx^k}[h(x)]\right) g(x),$$

the differential transform of the k-th order derivative of the product of the two functions can be obtained as follows:

$$F(k) = \frac{1}{k!} \left[\frac{d^k}{dx^k}[g(x)h(x)] \right]_{x=x_0}$$

$$= \frac{1}{k!} \left[\left\{ h(x) \frac{d^k}{dx^k}[g(x)] + \binom{k}{1} \frac{d}{dx}[h(x)] \frac{d^{k-1}}{dx^{k-1}}[g(x)] + \binom{k}{2} \frac{d^2}{dx^2}[h(x)] \frac{d^{k-2}}{dx^{k-2}}[g(x)] + \cdots \right.\right.$$

$$\left.\left. + \binom{k}{k-1} \frac{d^{k-1}}{dx^{k-1}}[h(x)] \frac{d}{dx}[g(x)] + \left(\frac{d^k}{dx^k}[h(x)]\right) g(x) \right\} \right]_{x=x_0}.$$

The last expression can also be rewritten as

$$F(k) = \frac{1}{k!} \left[h(x) \frac{d^k}{dx^k}[g(x)] \right]_{x=x_0} + \frac{1}{(k-1)!} \left[\frac{d}{dx}[h(x)] \frac{d^{k-1}}{dx^{k-1}}[g(x)] \right]_{x=x_0}$$

$$+\frac{1}{2(k-2)!}\left[\frac{d^2}{dx^2}[h(x)]\frac{d^{k-2}}{dx^{k-2}}[g(x)]\right]_{x=x_0}+\cdots+\frac{1}{(k-1)!}\left[\frac{d^{k-1}}{dx^{k-1}}[h(x)]\frac{d}{dx}[g(x)]\right]_{x=x_0}$$

$$+\frac{1}{k!}\left[\left(\frac{d^k}{dx^k}[h(x)]\right)g(x)\right]_{x=x_0}$$

As a result, it can be rewritten as

$$F(k)=G(k)H(0)+G(k-1)H(1)+G(k-2)H(2)$$

$$+\cdots G(1)H(k-1)+G(0)H(k)$$

$$=\sum_{l=0}^{k}G(l)H(k-l).$$

Theorem II

Let be $m\in\mathbb{N}$. If $f(x)=x^m$, then

$$F(k)=\begin{cases}\binom{m}{k}{x_0}^{m-k}, & k<m\\ 1, & k=m\\ 0, & k>m\end{cases}$$

,where $F(k)$ is the differential transform of $f(x)$.

Proof.

First of all, in terms of the sign of $k-m$, let us examine the derivative of $f(x)$ as follows:

Case 1

If $k>m$, then $m-k$ is strictly negative integer. For this reason, $\binom{m}{k}=0$. Furthermore, we know that

$$\frac{d^k}{dx^k}(x^m)=\frac{m!}{(m-k)!}x^{m-k}.$$

From Eq.(4), the differential transform of the k-th order derivative of $f(x)$ can be obtained as follows:

$$F(k)=\frac{1}{k!}\left[\frac{d^kf(x)}{dx^k}\right]_{x=x_0}=\frac{1}{k!}\left[\frac{d^k}{dx^k}(x^m)\right]_{x=x_0}$$

$$=\frac{1}{k!}\left[\frac{m!}{(m-k)!}x^{m-k}\right]_{x=x_0}=\frac{m!}{k!\,(m-k)!}{x_0}^{m-k}$$

$$=\binom{m}{k}{x_0}^{m-k}=0.{x_0}^{m-k}=0.$$

Case 2

If $k=m$,

$$F(k)=\frac{1}{k!}\left[\frac{d^kf(x)}{dx^k}\right]_{x=x_0}=\frac{1}{k!}\left[\frac{d^k}{dx^k}(x^m)\right]_{x=x_0}$$

$$= \frac{1}{k!}\left[\frac{m!}{(m-k)!}x^{m-k}\right]_{x=x_0} = \frac{m!}{k!\,(m-k)!}{x_0}^{m-k}$$

$$= \binom{m}{k}{x_0}^{m-k} = \binom{m}{m}{x_0}^{m-m} = 1.1 = 1.$$

Case 3

If $k < m$, then

$$F(k) = \frac{1}{k!}\left[\frac{d^k f(x)}{dx^k}\right]_{x=x_0} = \frac{1}{k!}\left[\frac{d^k}{dx^k}(x^m)\right]_{x=x_0}$$

$$= \frac{1}{k!}\left[\frac{m!}{(m-k)!}x^{m-k}\right]_{x=x_0} = \frac{m!}{k!\,(m-k)!}{x_0}^{m-k}$$

$$= \binom{m}{k}{x_0}^{m-k}.$$

Thus, from Cases (1)-(3) we have

$$F(k) = \begin{cases} \binom{m}{k}{x_0}^{m-k}, & k < m \\ 1, & k = m \\ 0, & k > m. \end{cases}$$

In the case of $x_0 = 0$, from the previous one we have

$$F(k) = \delta(k-m),$$

where

$$\delta(k-m) = \begin{cases} 1 & k = m \\ 0 & k \neq m. \end{cases}$$

Theorem III

If $w(u(x)) = \exp(u(x))$, then

$$W(k) = \begin{cases} \exp(U(0)), & k = 0 \\ \sum_{m=0}^{k-1} \frac{m+1}{k} U(m+1)W(k-m-1), & k \geq 1. \end{cases}$$

Proof.

Choosing $x_0 = 0$, from Eq.(4), for $k = 0$, we get

$W(0) = \frac{1}{0!}\left[\frac{d^0 \exp(u(x))}{dx^0}\right]_{x_0=0} = \exp\big(u(0)\big)$ and $U(0) = \frac{1}{0!}\left[\frac{d^0 u(x)}{dx^0}\right]_{x_0=0} = u(0).$

Thus, for $k = 0$, we get

$$W(0) = \exp(U(0)). \tag{7}$$

Now, taking the differentiation of $w(u(x)) = \exp(u(x))$ with respect to x, we get:

$$\frac{dw(u(x))}{dx} = \exp(u(x))\frac{d}{dx}(u(x)) = w(u(x))\frac{d}{dx}(u(x)). \tag{8}$$

Application of the differential transform to both sides of Eq. (8) gives:

$$(k+1)W(k+1) = \sum_{m=0}^{k}(m+1)U(m+1)W(k-m).$$

Replacing $k+1$ by k gives:

$$W(k) = \sum_{m=0}^{k-1}\frac{(m+1)}{k}U(m+1)W(k-m-1), \quad k \geq 1. \tag{9}$$

Combining Eqs. (7) and (9), we obtain the recursive relationship for calculating the T-function of $w(u(x)) = \exp(u(x))$:

$$W(k) = \begin{cases} \exp U(0), & k = 0 \\ \sum_{m=0}^{k-1}\frac{m+1}{k}U(m+1)W(k-m-1), & k \geq 1. \end{cases}$$

2.2. The solution to the problem (1)-(2)

Taking the differential transform of both sides of Eq. (1), the following recurrence relation is obtained:

$$\frac{(k+2)!}{k!}U(k+2) - \lambda\frac{(k+1)!}{k!}U(k+1) + \lambda\mu\sum_{l=0}^{k}[\beta\delta(l) - U(l))W(k-l)] = 0$$

or

$$(k+1)(k+2)U(k+2) - \lambda(k+1)U(k+1) + \lambda\mu\sum_{l=0}^{k}[\beta\delta(l) - U(l))W(k-l)] = 0.$$

The former one is rewritten as follows:

$$U(k+2) = \frac{1}{(k+1)(k+2)} \times \left(\lambda(k+1)U(k+1) + \lambda\mu\sum_{l=0}^{k}[U(l) - \beta\delta(l))W(k-l)]\right), k \geq 0, \tag{10}$$

where $\delta(l)$ is a function such that $\delta(l) = \begin{cases} 1 & l = 0 \\ 0 & l \neq 0 \end{cases}$, the differential transform of $\beta = \beta.x^0$, $U(k)$ is the differential transform of $u(x)$, and $W(k)$ is the differential transform of $\exp(u(x))$ are given as follows:

$$W(k) = \begin{cases} \exp U(0), & k = 0 \\ \sum_{m=0}^{k-1}\frac{m+1}{k}U(m+1)W(k-m-1), & k \geq 1. \end{cases}$$

Choosing $x_0 = 0$ and using Eq.4, the differential transform of the first one of boundary conditions given in Eq. (2) is given as follows:

$$u'(0) = \lambda u(0) \Rightarrow \left[\frac{du(x)}{dx}\right]_{x_0=0} = 1!\,U(1) = \lambda[u(x)]_{x_0=0} = \lambda 0!\,U(0)$$

$$\Rightarrow U(1) - \lambda U(0) = 0$$

As to the differential transform of the second one of boundary conditions given in Eq. (2), choosing $x_0 = 0$ and taking the first derivative of Eq.(6), we get

$$u'(x) = \sum_{k=1}^{N} kU(k)\,x^k \Rightarrow u'(1) = \sum_{k=1}^{N} kU(k) = 0 \Rightarrow \sum_{k=1}^{N} kU(k) = 0$$

That is, the differential transform of the conditions given in Eq.(2) are as follows

$$U(1) - \lambda U(0) = 0, \sum_{k=1}^{N} kU(k) = 0. \tag{11}$$

Furthermore, from Eq.(4),

$$U(0) = \frac{1}{0!}\left[\frac{d^0 u(x)}{dx^0}\right]_{x_0=0} = [u(x)]_{x_0=0} = u(0).$$

Now, since u(0) is not known, called missing initial condition, put

$$U(0) = A. \tag{12}$$

For this reason, from the first one of Eq. (11), we find that

$$U(1) = \lambda A. \tag{13}$$

At $k = 0$ and substituting Eq.(12) and Eq.(13) into Eq.(10), we have

$$U(2) = \frac{A\lambda^2}{2} + \frac{1}{2}Ae^A\lambda\mu - \frac{1}{2}e^A\beta\lambda\mu. \tag{14}$$

At $k = 1$ and substituting Eqs.(12),(13) and (14) into Eq.(10), we have

$$U(3) = \frac{A\lambda^3}{6} + \frac{1}{3}Ae^A\lambda^2\mu + \frac{1}{6}A^2e^A\lambda^2\mu - \frac{1}{6}e^A\beta\lambda^2\mu - \frac{1}{6}Ae^A\beta\lambda^2\mu.$$

Following the same procedure, we calculate up to N-th term $U(N)$ and substituting from $U(0)$ to $U(N)$ into Eq. (6), we obtain a few-term solution as follows:

$$u(x) = A + Ax\lambda + x^2\left(\frac{A\lambda^2}{2} + \frac{1}{2}Ae^A\lambda\mu - \frac{1}{2}e^A\beta\lambda\mu\right)$$
$$+x^3\left(\frac{A\lambda^3}{6} + \frac{1}{3}Ae^A\lambda^2\mu + \frac{1}{6}A^2e^A\lambda^2\mu - \frac{1}{6}e^A\beta\lambda^2\mu - \frac{1}{6}Ae^A\beta\lambda^2\mu\right) + \cdots, \tag{15}$$

Similarly, substituting from $U(0)$ to $U(N)$ into the second one of Eq. (11), we obtain

$$U(1) + 2U(2) + 3U(3) + \cdots = 0,$$

namely,

$$A\lambda + A\lambda^2 + Ae^A\lambda\mu - e^A\beta\lambda\mu + \frac{A\lambda^3}{3} + \frac{2}{3}Ae^A\lambda^2\mu + \frac{1}{3}A^2e^A\lambda^2\mu - \frac{1}{3}e^A\beta\lambda^2\mu - \frac{1}{3}Ae^A\beta\lambda^2\mu + \cdots = 0. \quad (16)$$

The constant A can be evaluated from Eq. (16), numerically for the selected values of λ, μ and β. If the values of λ, μ and β are taken to be 5, 0.05 and 0.53, respectively, the constant A was found to be 0.00521611 by taking $N = 20$. Therefore, we get the following series solution

$$\begin{aligned} u(x) = {} & 0.00521611 + 0.0260805x - 0.000739718x^2 - 0.00071375x^3 - 0.000889043x^4 - 0.00089357x^5 \\ & - 0.000748412x^6 - 0.000537325x^7 - 0.000337575x^8 - 0.00018529x^9 - 0.0000947654x^{10} \\ & - 0.0000433045x^{11} - 0.0000181387x^{12} - 7.0119 \times 10^{-6}x^{13} - 2.51586 \times 10^{-6}x^{14} \\ & - 8.41679 \times 10^{-7}x^{15} - 2.63443 \times 10^{-7}x^{16} - 7.7279 \times 10^{-8}x^{17} - 2.12247 \times 10^{-8}x^{18} \\ & - 5.42369 \times 10^{-9}x^{19} - 1.26638 \times 10^{-9}x^{20} + O(x^{21}). \end{aligned}$$

3. Numerical Results

This section includes our numerical experiments for the solution of the problem (1)–(2) based on the present method. In particular, we consider appropriate selections of the parameters λ, μ and β, in order to guarantee the existence of a unique solution. We start by reporting the results for the case $\lambda = 5, \mu = 0.7, \beta = 0.8$ whose existence and uniqueness of solutions are shown in [5].

Table II. Numerical solutions for $\lambda = 5, \mu = 0.7, \beta = 0.8$ using $N = 21$

x	Present method	Method of [3]
0.0	0.10164624270973075803	0.10164623106412275851
0.1	0.15160802174765053429	0.15160800244418513970
0.2	0.19969085827917187892	0.19969082598774598630
0.3	0.24564769362604130242	0.24564763919882120986
0.4	0.28919561887003542022	0.28919552652683175159
0.5	0.32997403262441354909	0.32997387500728383184
0.6	0.36746695397036449604	0.36746668342588013969
0.7	0.40086194130361912924	0.40086147462729197629
0.8	0.42879644411667916515	0.42879563852127257524
0.9	0.4489041236159168613	0.44890277089707031201
1.0	0.45700728808538226833	0.45700543763742257810

In Table II, we display our numerical results using 21 iterations and compare them with that of the obtained results in [3] for the same iteration number. The second case that we will consider is $\lambda = 5, \mu = 0.05, \beta = 0.53$ whose existence and uniqueness of the solution are discussed in [5]. Table III depicts our results for this case and compare them with that of the obtained results in [3] for 9 iterations.

Table III. Numerical solutions for $\lambda = 5, \mu = 0.05, \beta = 0.53$ using $N = 9$

x	Present method	Method of [3]
0.0	0.00521358107832754769	0.00521610631917866806
0.1	0.00781178436241308435	0.00781594990560462475
0.2	0.01038827332747585021	0.01039514976995603891
0.3	0.01293300159161900505	0.01294435771748241589
0.4	0.01542939714475057879	0.01544814585192753329
0.5	0.01785016461112156824	0.01788103688272135216
0.6	0.02015055366278014487	0.02020094227138412933
0.7	0.02225781839224119998	0.02233831543368271460
0.8	0.02405515194132944526	0.02417822175475618635
0.9	0.02535786662489987117	0.02553069994644663735
1.0	0.02587900218297151111	0.02508176937417854529

For the first case, our results match with, at least, five decimal places of the values obtained in [3] while our results match with, at least, three decimal places of the values obtained in [3] for the second case.

Table IV. Numerical solutions and comparison for $\lambda = 10, \mu = 0.02, \beta = 3$ using $N = 11$

x	Present method	Method of [3]	Method of [6]	Method of [7]
0.0	0.0060481652730214469	0.0060483739097476077	0.006048	0.006048
0.2	0.0181914018945969064	0.0181929364878594473	0.018192	0.018192
0.4	0.0304134413420211330	0.0304246702566782983	0.030424	0.030424
0.6	0.0425905527398581715	0.0426691183249326775	0.042669	0.042669
0.8	0.054280015400578142	0.0543716533646849943	0.054371	0.054371
1.0	0.061404146374997812	0.0614587374322116238	0.061458	0.061458

Finally, we consider one more case that is available for comparison in the literature with various numerical methods. Table IV reports our results for the case $\lambda = 10, \mu = 0.02, \beta = 3$. Existence and uniqueness of the solution are guaranteed by contraction mapping principle [6]. Table IV depicts our results for this case and compare them with those of the obtained results in [3] for 11 iterations and the solutions obtained in [6] and [7]. For this case, our results match with, at least, three decimal places of the values obtained in [3].

In Figure 1, we present the convergence of calculated missing condition A with increasing N.

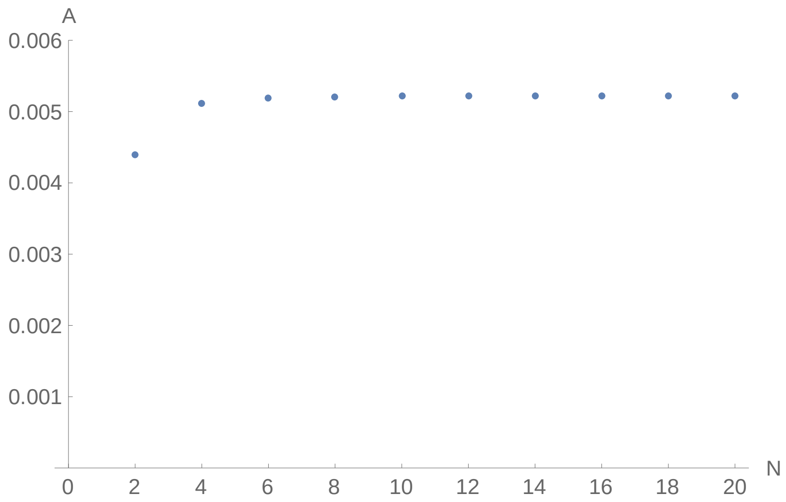

Fig.1. Variation of A with N for the case $\lambda = 5, \mu = 0.05, \beta = 0.53$.

Moreover, since there is no exact solution of this problem, we instead investigate the absolute residual error function, which is the measure of how well the numerical solution satisfies the original problem (1)-(2). The absolute residual error function is

$$|\mathrm{ER}_N(x)| = |u_N''(x) - \lambda u_N'(x) + \lambda\mu(\beta - u_N(x))\exp(u_N(x))|, 0 \le x \le 1.$$

In Figure 2, we present the absolute residual error function $|\mathrm{ER}_{20}(x)|$ for the case $\lambda = 5, \mu = 0.05, \beta = 0.53$.

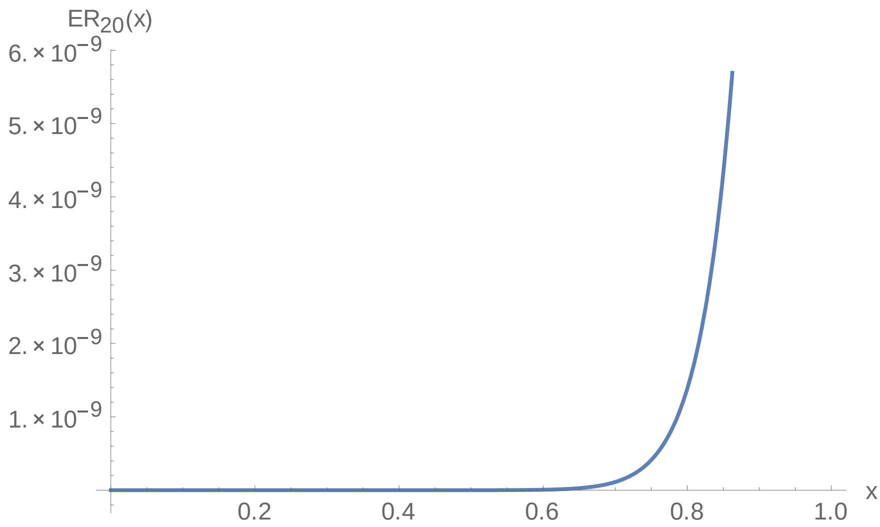

Fig.2. Absolute residual error function $|\mathrm{ER}_{20}(x)|$.

Conclusions

In this work, differential transform method is implemented to estimate the steady-state solution of the irreversible exothermic chemical reaction that occurs in adiabatic tubular chemical reactor. One main advantage of the present method is that the nonlinear structure is handled without the need for restrictive assumptions.

The convergence of the present method is shown numerically. The computed residual error function demonstrates the accuracy of the suggested method.

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