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Ethanol and Acetaldehyde in a fixed bed laboratory reactor by the Adomian decomposition method

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Abstract
In this paper, we will obtain the analytical approximations solution for a system of two coupled nonlinear differential equations that represent the concentration of ethanol and acetaldehyde by using the Adomian decomposition method combined with the Duan – Rach modified recursion scheme. This system models that determine the kinetic study of ethanol combustion on a Mn/Cu catalyst and formulating feasible reaction rate expressions with their corresponding kinetic parameters. The obtain solution have been analyzing that demonstrate the rapid rate of convergence of our sequence of analytic approximate solutions without recourse to comparisons with an alternate solution technique. The Adomian decomposition method yields a rapidly convergent, easily computable and readily verifiable sequence of analytic approximations that are convenient for parametric simulations.

Keywords
Adomian Decomposition Method (ADM), Numerical simulation, Ethanol, Acetaldehyde, mathematical modeling.

AMS Subject Classification
41A60, 65L06, 92E20, 03C50.

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Contents

1. Introduction

One of the major contributors to air pollution is emission of volatile organic compounds (VOCs) from many industrial processes [5, 6, 14, 29]. In printing industries emitted two of VOC's solvent namely ethanol and acetaldehyde [13]. This type of VOC's are destroyed from the catalyst combustion [13]. Morales et.al.,[15] has been formulated an efficient catalyst of Mn and Cu by co-precipitation method. Morales et al.[15] and Pramparo [16] discussed the preparation and physical characterization of the catalyst. M.A. Campesi et.al.,[4],developed a mathematical model that describes ethanol and acetaldehyde molar concentrations inside the catalyst particle.

In this work, we shall systematically obtain the approximate solution by the Adomian decomposition method [1–3, 12, 17, 26] combine with the Duan - Rach modified recursion scheme [7, 9, 21]. Also we represent the graphs of error analysis of our approximate solutions for the reason the rate of convergence of our solutions and the maximal error remainder parameters instead of comparison to an alternate solution technique alone.We observe that the Adomian decomposition method has been efficiently used to solve a wide variety of nonlinear problems in engineering and science [8, 10, 11, 19, 20, 28], especially including several in theoretical chemistry [18, 22–25, 27].

2. Problem Description

M.A. Campesi et.al.[4], a mathematical model that relates the ethanol and acetaldehyde molar concentrations inside the catalyst particle is established as nonlinear differential equation as follows [4]:

$$D_{ef,Et}\left[\frac{1}{z^2}\frac{d}{dz}\left(z^2\frac{dC_{Et}}{dz}\right)\right]=r_1 \tag{2.1}$$

$$D_{ef,Ac}\left[\frac{1}{z^2}\frac{d}{dz}\left(z^2\frac{dC_{Ac}}{dz}\right)\right]=r_2-r_1 \tag{2.2}$$

Subject to mixed sets of Neumann and Dirichlet boundary conditions[4]:

$$z=R\ ;\ \ C_{Et}=C_{Et}^b,\ \ C_{Ac}=C_{Ac}^b \tag{2.3}$$

$$z=0\ ;\ \ \frac{dC_{Et}}{dz}=0,\ \ \frac{dC_{Ac}}{dz}=0 \tag{2.4}$$

The reaction rate r_1 and r_2 are as follows [4]:

$$r_1=\frac{k_{ref_1}e^{\left[-(E_1/R_G)((1/T)-(1/T_{ref}))\right]C_{Et}}}{1+K_{C_{Et}}C_{Et}+K_{C_{Ac}}C_{Ac}} \tag{2.5}$$

$$r_2=\frac{k_{ref_2}e^{\left[-(E_2/R_G)((1/T)-(1/T_{ref}))\right]C_{Ac}}}{1+K_{C_{Et}}C_{Et}+K_{C_{Ac}}C_{Ac}} \tag{2.6}$$

Where the functions C_{Et} and C_{Ac} denote the molar concentrations of ethanol and acetaldehyde inside the catalyst particle, $D_{ef,Et}$ and $D_{ef,Ac}$ are the effective diffusivities of ethanol and acetaldehyde, T_{ref} is the reference temperature, R_G is a gas constant, $K_{C_{Et}}$ and $K_{C_{Ac}}$ are the adsorption equilibrium constant of ethanol and acetaldehyde respectively and E_1 and E_2 are activation energies respectively.
Introducing dimensionless variables from the above system of nonlinear equations:

$$u=\frac{C_{Et}}{C_{Et}^b};w=\frac{C_{Ac}}{C_{Ac}^b};x=\frac{z}{R};\beta_1=\frac{k_{ref_1}R^2}{D_{ef,Et}};\beta_2=\frac{k_{ref_2}R^2}{D_{ef,Et}};$$
$$\beta_3=\frac{k_{ref_1}C_{Et}^bR^2}{D_{ef,Ac}C_{Ac}^b};\alpha_1=k_{C_{Et}}C_{Et}^b;\alpha_2=k_{C_{Ac}}C_{Ac}^b;$$
$$\phi_1=e^{\left[-\frac{E_1}{R_G}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]};\phi_2=e^{\left[-\frac{E_2}{R_G}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]} \tag{2.7}$$

The corresponding dimension non-linear equations (2.1) - (2.6) can be written as:

$$\frac{d^2u}{dx^2}+\frac{2}{x}\frac{du}{dx}=F_1\left(u(x),w(x)\right) \tag{2.8}$$

$$\frac{d^2w}{dx^2}+\frac{2}{x}\frac{dw}{dx}=F_2\left(u(x),w(x)\right) \tag{2.9}$$

Subject to the boundary conditions[4]:

$$x=1\ ;\ \ u(1)=1,\ \ w(1)=1 \tag{2.10}$$

$$x=0\ ;\ \ \frac{du}{dx}=0,\ \ \frac{dw}{dx}=0 \tag{2.11}$$

where the functions $u(x)$ and $w(x)$ are the concentration of the ethanol and acetaldehyde respectively, x is the dimensional distance, and the system nonlinearities are

$$F_1\left(u(x),w(x)\right)=\beta_1\phi_1 f_1\left(u(x),w(x)\right) \tag{2.12}$$

$$F_2\left(u(x),w(x)\right)=\beta_2\phi_2 f_2\left(u(x),w(x)\right)-\beta_3\phi_1 f_1\left(u(x),w(x)\right) \tag{2.13}$$

where

$$f_1\left(u(x),w(x)\right)=\frac{u(x)}{1+\alpha_1u(x)+\alpha_2w(x)} \tag{2.14}$$

$$f_2\left(u(x),w(x)\right)=\frac{w(x)}{1+\alpha_1u(x)+\alpha_2w(x)} \tag{2.15}$$

3. Mathematical Procedures

In this section, ADM method has been investigated:

3.1 Modified recursion scheme using the ADM

To explain the basic ideas of this method, we consider the following Lane – Emden equation

$$\frac{d^2z}{dr^2}+\frac{2}{r}\frac{dz}{dr}=N\left(z(r)\right) \tag{3.1}$$

Subject to Neumann and Dirichlet boundary condition

$$z'(0)=0\ ;\ \ z(1)=\beta \tag{3.2}$$

where $N(z(r))$ is a nonlinear function of $z(r)$. We propose the new differential operator $Lv= r^{-1}\frac{d^2}{dr^2}rv$, Eqn.(3.1) can be written as

$$Lz(r)=N\left(z(r)\right) \tag{3.3}$$

Applying $L^{-1}v(x)=\int_0^x\left(y-\frac{y^2}{x}\right)v(y)dy$ the inverse operator to both sides of Eqn.(3.3) yields

$$z(r)=z(0)+L^{-1}N\left(z(r)\right) \tag{3.4}$$

It is a non-linear Volterra integral equations with undetermined – constants of integration z(0) as an intermediate step. Denote

$$L_1^{-1}v(x)=\left[L^{-1}v(x)\right]_{x=1}=\int_0^1\left(y-y^2\right)v(y)dy \tag{3.5}$$

Next, we apply the corresponding inverse linear operator $L_1^{-1}(\cdot)$ to both sides of Eqn.(3.4) and substituting the boundary condition $z(1)=\beta$. we have

$$z(0)=\beta-L_1^{-1}N\left(z(r)\right) \tag{3.6}$$

Substituting Eqn.(3.6) into Eqn.(3.4), we obtain the equivalent nonlinear Fredholm – Volterra integral equation without any undetermined constants of integration as

$$z(0)=\beta-L_1^{-1}N\left(z(r)\right)+L^{-1}N\left(z(r)\right) \tag{3.7}$$

Applying the Adomian decomposition series and the series of the two-variable Adomian polynomials [2, 3, 7], we have

$$z(r)=\sum_{n=0}^{\infty}z_n(r) \tag{3.8}$$

$$\text{and}\quad N\left(z(r)\right)=\sum_{n=0}^{\infty}A_{1,n}(r) \tag{3.9}$$

where the two - variable Adomian polynomials $A_{1,n}(y)$ are defined as

$$A_{1,n}(r) = \frac{1}{n!}\frac{d^n}{d\lambda^n} z\left(\sum_{n=0}^{\infty}\lambda^n z_n(r)\right)\Bigg|_{\lambda=0} \tag{3.10}$$

Upon substitution of the decompositions Eqn.(3.8) and (3.9) into Eqn.(3.7) , we obtain

$$\begin{aligned}\sum_{n=0}^{\infty} z_n(r) =& \beta - \int_0^1 (r-r^2)\sum_{n=0}^{\infty} A_{1,n}(r)dr \\ &+ \int_0^x \left(r-\frac{r^2}{x}\right)\sum_{n=0}^{\infty} A_{1,n}(r)dr \end{aligned}\tag{3.11}$$

We set the system of two-coupled Duan-Rach modified recursion schemes as [2]:

$$z_0(x) = \beta \tag{3.12}$$

$$\begin{aligned} z_{n+1}(r) =& -\int_0^1 (r-r^2)\sum_{n=0}^{\infty} A_{1,n}(r)dr \\ &+ \int_0^x \left(r-\frac{r^2}{x}\right)\sum_{n=0}^{\infty} A_{1,n}(y)dy,\ n\geq 0 \end{aligned}\tag{3.13}$$

Then we obtain the approximate solution functions as defined by Adomian decomposition method is

$$\varphi_{m+1}(x) = \sum_{n=0}^{\infty} z_n(x) \tag{3.14}$$

If the exact solution is unknown, we compute the following error remainder functions and the maximal error remainder parameter as the error analysis for the sequence of approximate solution. The error remainder functions and the maximal error remainder parameter are

$$ER_n(r) = \frac{d^2\varphi_n}{dr^2} + \frac{2}{r}\frac{d\varphi_n}{dr} - N(\varphi_n(r)) \tag{3.15}$$

$$\text{and}\quad MER_n(r) = \max_{0\leq r\leq 1} |ER_n(r)| \tag{3.16}$$

which are a measure of how well the sequence of solution approximations satisfy the original nonlinear differential equation.

4. Application of Described Manners in the Issue

4.1 Adomian decomposition method (ADM)

In this section, we will apply the ADM to nonlinear ordinary differential Eqns. (2.8) – (2.11). First of all, we approximate $u(x)$ and $w(x)$ as

$$\begin{aligned} u(x) =& 1 - \int_0^1 (r-r^2) F_1(u(y),w(y))\,dy \\ &+ \int_0^x \left(y-\frac{y^2}{x}\right) F_1(u(y),w(y))\,dy \end{aligned}\tag{4.1}$$

$$\begin{aligned} w(x) =& 1 - \int_0^1 (r-r^2) F_2(u(y),w(y))\,dy \\ &+ \int_0^x \left(y-\frac{y^2}{x}\right) F_2(u(y),w(y))\,dy \end{aligned}\tag{4.2}$$

Next we apply the respective Adomian decomposition series

$$u(x) = \sum_{n=0}^{\infty} u_n(x), \quad w(x) = \sum_{n=0}^{\infty} w_n(x) \tag{4.3}$$

and the nonlinear function are

$$F_1(u(x),w(x)) = \sum_{n=0}^{\infty} A_{1,n}(y), F_2(u(x),w(x)) = \sum_{n=0}^{\infty} A_{2,n}(y) \tag{4.4}$$

$$f_1(u(x),w(x)) = \sum_{n=0}^{\infty} B_{1,n}(y), f_2(u(x),w(x)) = \sum_{n=0}^{\infty} B_{2,n}(y) \tag{4.5}$$

where the two - variable Adomian polynomials satisfy

$$A_{1,n} = \beta_1\phi_1 B_{1,n},\quad A_{2,n} = \beta_2\phi_2 B_{2,n} - \beta_3\phi_1 B_{1,n} \tag{4.6}$$

$$\begin{aligned} B_{1,0} &= \frac{u_0}{1+\alpha_1 u_0 + \alpha_2 w_0}, \\ B_{1,1} &= \frac{u_1 + (1-\alpha_1)u_0 u_1 + \alpha_2(u_1 w_0 - \alpha_2 u_0 w_1)}{(1+\alpha_1 u_0+\alpha_2 w_0)^2}\cdots\cdots \end{aligned}\tag{4.7}$$

$$\begin{aligned} B_{2,0} &= \frac{w_0}{1+\alpha_1 u_0 + \alpha_2 w_0}, \\ B_{2,1} &= \frac{w_1 + (1-\alpha_2)w_0 w_1 + \alpha_1(u_0 w_1 - \alpha_2 u_1 w_0)}{(1+\alpha_1 u_0+\alpha_2 w_0)^2}\cdots\cdots \end{aligned}\tag{4.8}$$

For convenience, we use MATHEMATICA code generating the two-variable Adomian polynomials of the general bivariate function $f(u,w)$ is listed in the Appendix. From this, we list first five two-variable Adomian polynomials of the general bivariate function $f(u,w)$ with the decompositions $u(x) = \sum_{n=0}^{\infty} u_n(x)$, $w(x) = \sum_{n=0}^{\infty} w_n(x)$ as follows,

$$\begin{aligned} A_0 =& f(u_0,v_0), \\ A_1 =& v_1 f^{(0,1)} + u_1 f^{(1,0)}, \\ A_2 =& v_2 f^{(0,1)} + \frac{u_1 v_1^2}{2} f^{(0,2)} + u_2 f^{(1,0)} + u_1 v_1 f^{(1,1)} \\ &+ \frac{u_1^2}{2} f^{(2,0)}, \\ A_3 =& v_3 f^{(0,1)} + v_1 v_2 f^{(0,2)} + \frac{1}{6} v_1^3 f^{(0,3)} + u_3 f^{(1,0)} \\ &+ (u_2 v_1 + u_1 v_2) f^{(1,1)} + \frac{1}{2} u_1 v_1^2 f^{(1,2)} + u_1 v_1 f^{(2,0)} \\ &+ \frac{1}{2} u_1^2 v_1 f^{(2,1)} + \frac{1}{6} u_1^3 f^{(3,0)}, \end{aligned}$$

$$
\begin{aligned}
A_4 =& v_4 f^{(0,1)} + \left(\frac{v_2^2}{2} + v_1 v_3\right) f^{(0,2)} + \frac{v_1^2 v_2}{2} f^{(0,3)} \\
&+ \frac{v_1^4}{24} f^{(4,0)} + u_4 f^{(1,0)} + (u_3 v_1 + u_2 v_2 + u_1 v_3) f^{(1,1)} \\
&+ \left(\frac{1}{2} v_1^2 u_1 + u_2 v_1 v_2\right) f^{(1,2)} + \frac{u_1 v_1^3}{6} f^{(1,3)} \\
&+ \left(u_1 u_3 + \frac{u_2^2}{2}\right) f^{(2,0)} + \left(u_1 u_2 v_1 + \frac{u_1^2 v_2}{2}\right) f^{(2,1)} \\
&+ \frac{u_1^2 v_1^2}{4} f^{(2,2)} + \frac{u_1^2 u_2}{2} f^{(3,0)} + \frac{u_1^3 v_1}{6} f^{(3,0)} \\
&+ + \frac{u_1^4}{24} f^{(4,0)}
\end{aligned}
$$

where the notation $f^{(m,n)} = f^{(m,n)}(u_0, v_0) = \frac{\partial^{m+n} f}{\partial u^m \partial v^n}(u_0, v_0)$. Upon substitution of the decompositions Eqn.(4.3) and (4.4) into Eqns.(4.1) and (4.2) , we obtain

$$\sum_{n=0}^{\infty} u_n(x) = 1 - L_1^{-1} \sum_{n=0}^{\infty} A_{1,n}(x) + L_1 \sum_{n=0}^{\infty} A_{1,n}(x) \quad (4.9)$$

$$\sum_{n=0}^{\infty} w_n(x) = 1 - L_1^{-1} \sum_{n=0}^{\infty} A_{2,n}(x) + L_1 \sum_{n=0}^{\infty} A_{2,n}(x) \quad (4.10)$$

We establish the system of coupled Duan-Rach modified recursion schemes

$$
\begin{aligned}
&u_0(x) = 1 \\
&u_{n+1}(x) = -L_1^{-1} \sum_{n=0}^{\infty} A_{1,n}(x) + L_1 \sum_{n=0}^{\infty} A_{1,n}(x), \ n \geq 0
\end{aligned}
\quad (4.11)
$$

$$
\begin{aligned}
&w_0(x) = 1 \\
&w_{n+1}(x) = -L_1^{-1} \sum_{n=0}^{\infty} A_{2,n}(x) + L_1 \sum_{n=0}^{\infty} A_{2,n}(x), \ n \geq 0
\end{aligned}
\quad (4.12)
$$

Next, we list the first calculated solution components as

$$u_1(x) = \frac{\beta_1 \phi_1}{6(1 + \alpha_1 + \alpha_2)} \left(x^2 - 1\right) \quad (4.13)$$

$$w_1(x) = \frac{\beta_2 \phi_2 - \beta_3 \phi_1}{6(1 + \alpha_1 + \alpha_2)} \left(x^2 - 1\right) \quad (4.14)$$

Then we obtain the two approximate solutions as

$$u_{m+1}(x) = \sum_{n=0}^{\infty} u_n(x), \quad w_{m+1}(x) = \sum_{n=0}^{\infty} w_n(x), \ m \geq 0. \quad (4.15)$$

5. Numerical Simulations

First, we assign $\alpha_1 = 20$, $\alpha_2 = 10$ in Eqn.(4.15). Further, we examine the error remainder functions and the maximal error remainder parameter for $\beta_1 = \beta_2 = \phi_1 = \phi_2 = 0.1$, $\beta_3 = 0.5$.

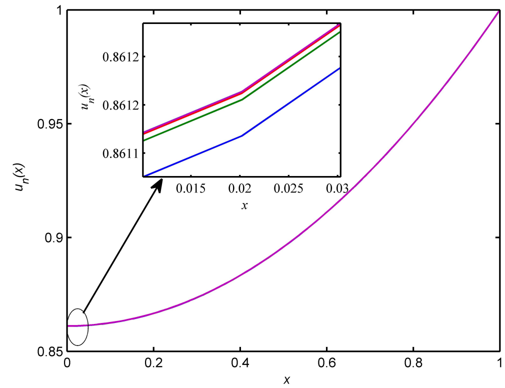

Figure 1. Plots of the approximate solutions $u_n(x)$ verse x for $n = 2$ to 6

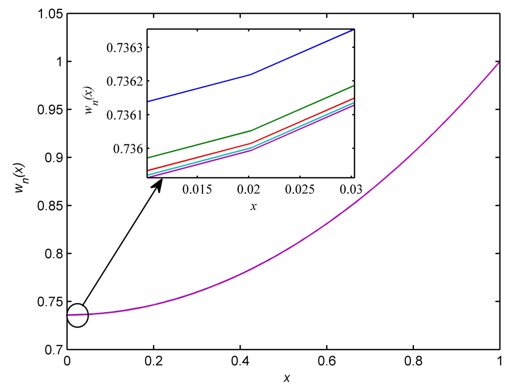

Figure 2. Plots of the approximate solutions $w_n(x)$ verse x for $n = 2$ to 6

From these figures, we represents five curves nearly overlap of the approximate solutions $u_n(x)$ and $w_n(x)$ versus x for $n = 2$ to 6, respectively. We consider the error remainder functions

$$ER_n^{<1>}(r) = \frac{d^2 u_n}{dx^2} + \frac{2}{x}\frac{du_n}{dx} - F_1\left(u_n(x), w_n(x)\right), \quad (5.1)$$

$$ER_n^{<2>}(r) = \frac{d^2 w_n}{dx^2} + \frac{2}{x}\frac{dw_n}{dx} - F_2\left(u_n(x), w_n(x)\right) \quad (5.2)$$

$$
\begin{aligned}
&\text{and } MER_n^{<1>}(x) = \max_{0 \leq x \leq 1} \left|ER_n^{<1>}(x)\right|, \\
&MER_n^{<2>}(x) = \max_{0 \leq x \leq 1} \left|ER_n^{<2>}(x)\right|
\end{aligned}
\quad (5.3)
$$

From Eqns.(5.1) - (5.3) , we obtained the error remainder parameters $ER_n^{<1>}$ and $ER_n^{<2>}$ for $n = 2$ to 7 and these are displayed in figures 3 and 4. Also the maximal error remainder parameters $MER_n^{<1>}$ and $MER_n^{<2>}$ for $n = 2$ to 8. Table 1 represent the maximal error remainder parameters $MER_n^{<1>}$ and $MER_n^{<2>}$.

In addition, we examine the effects of the parameters α_i's; ϕ_i's; β_i's to the approximations solutions $u_n(x)$ and $w_n(x)$. Fig. 5 – 10 represents the effects of β_1, ϕ_1 and α_2 on the approximate solution $u_6(x)$ and the effects of β_2, ϕ_2 and α_2 on the approximate solution $u_6(x)$. From these, we conclude that the approximate solution of $u_6(x)$ increases with the increasing value of parameters β_2, ϕ_2 and α_2, the approximate solution of $u_6(x)$ are very strong for the decreasing value of β_2, ϕ_2, and increasing the value of α_2.

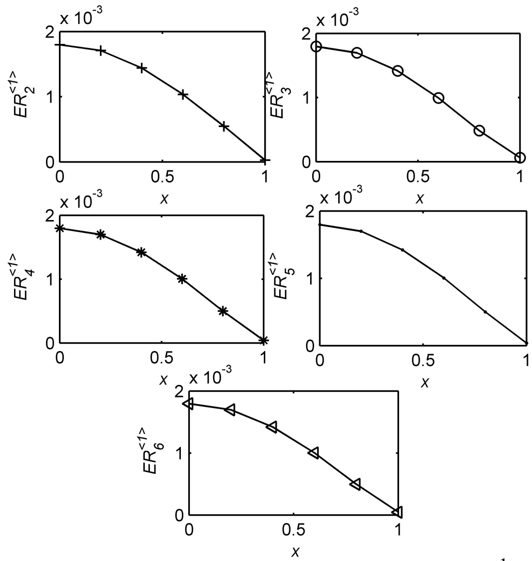

Figure 3. Plots of the error remainder functions $ER_n^{<1>}(x)$ verse x for n = 2 to 6

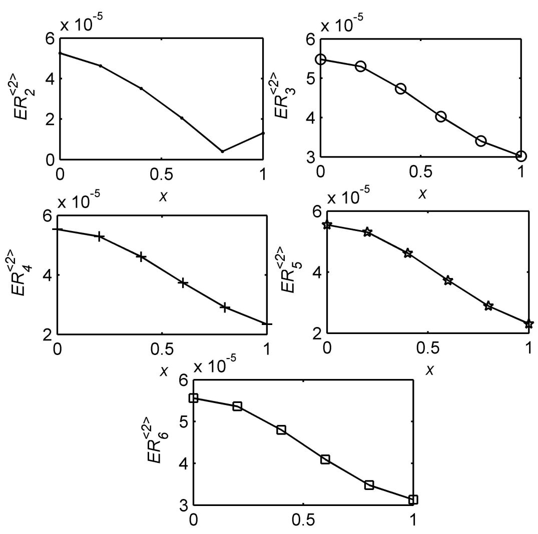

Figure 4. Plots of the error remainder functions $ER_n^{<2>}(x)$ verse x for n = 2 to 6

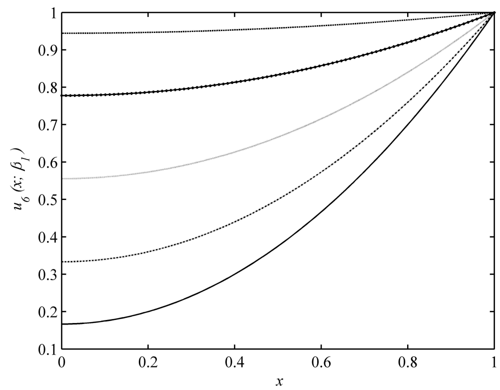

Figure 5. Effect of β_1 (= 1, 4, 8, 12, 15) on the approximate solution $u_6(x)$ verse x for different values of β_2 = 0.001, β_3 = α_1 = α_2 = ϕ_1 = ϕ_2 = 1.

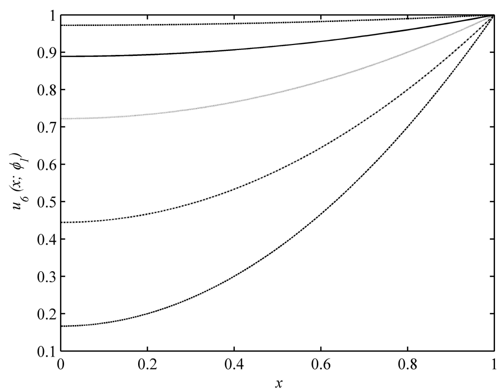

Figure 6. Effect of ϕ_1 (= 0.5, 2, 5, 10, 15) on the approximate solution $u_6(x)$ verse x for different values of β_1 = β_2 = β_3 = α_1 = α_2 = ϕ_2 = 1.

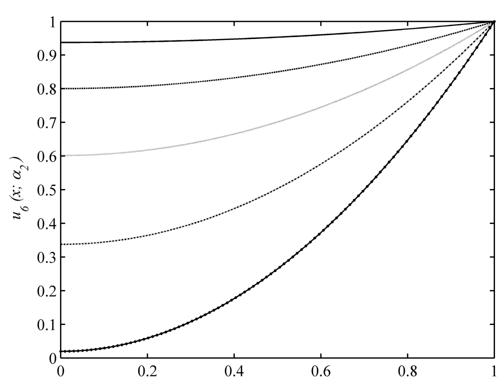

Figure 7. Effect of α_2 (= 0.01, 0.5, 1.5, 4, 15) on the approximate solution $u_6(x)$ verse x for different values of β_1 = 6, β_2 = β_3 = α_1 = ϕ_1 = 1, ϕ_2 = 0.01.

6. Conclusion

In this work, we have investigated the fixed bed laboratory reactor involved in a system of the Ethanol and Acetaldehyde. The system models that represent the kinetic study of ethanol combustion on a Mn/Cu catalyst in fixed bed laboratory reactor. The Adomian Decomposition method with the Duan-Rach modified recursion scheme have been used to solving the system of nonlinear differential equations and the work resulted approximation solution of the concentration of Ethanol and Acetaldehyde with a high level of accuracy. The evaluated approximations show enhancements over existing

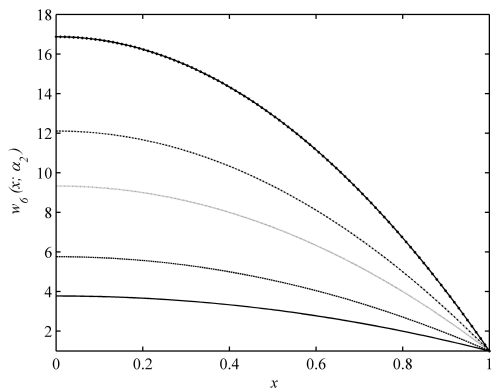

Figure 8. Effect of α_2 (= 0.1, 1, 2, 5, 10) on the approximate solution $w_6(x)$ verse x for different values of β_1 = 1, β_2 = 0.001, β_3 = 100, α_1 = ϕ_2 = 1, ϕ_1 = 2.

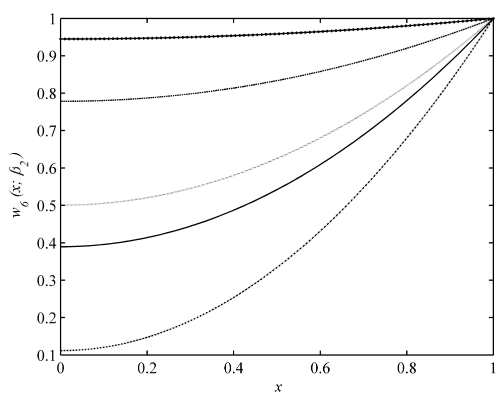

Figure 9. Effect of β_2 (= 0.1, 1, 2, 5, 10) on the approximate solution $w_6(x)$ verse x for different values of β_1 = 1, β_3 = 0.001, α_1 =1, α_2 = 100, ϕ_1 = 2, ϕ_2 = 1.

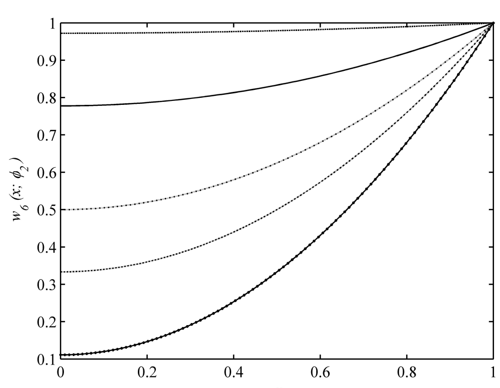

Figure 10. Effect of ϕ_2 (= 1.5, 5, 10, 13, 17) on the approximate solution $w_6(x)$ verse x for different values of β_1 = β_2 = β_3 = α_1 = α_2 = ϕ_1 = 1.

techniques where the minimal size of the obtained errors and the illustrated graphs emphasize these improvements.

Table 1. The Maximal error remainder parameters $MER_n^{<1>}$ and $MER_n^{<2>}$

n	$MER_n^{<1>}$	$MER_n^{<2>}$
2	0.001796042618	0.00005255255270
3	0.001796556434	0.00005480813514
4	0.001796650019	0.00005531323514
5	0.001796672451	0.00005549765676
6	0.001796671545	0.00005560060135

7. Appendix

MATHEMATICA code for the two-variable Adomian polynomials:

```
Adth1[M_]:=Module[,A[0]=f[Subscript[u,0],Subscript[v,0]];
For[n=1,n¡=M,n++,A[n]=1/n* Sum[(k+1)*
(Subscript[u, k+1]*D[A[n-1-k], Subscript[u,0]] +Subscript[v,
k+1]*D[A[n-1-k],Subscript[v, 0]]),k,0,n-1]];
Table[A[n],n,0,M]].
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