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Analytical and numerical solution of the nonlinear differential equation for self-igniting reaction diffusion systems: Mathematical modelling approach

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Abstract

Mathematical models of self-igniting reaction diffusion systems are discussed theoretically. The model comprises a system of reaction-diffusion equations that are nonlinearly connected. The efficient and easily accessible analytical technique AGM was used to solve the steady-state non-linear equations for a self-igniting reaction diffusion system. The proposed method's efficiency and accuracy will be tested against some of the widely used numerical approaches found in the literature Herein, we present the generalized approximate analytical solution for the concentration of gas reactant and temperature for the experimental values of heat of reaction, thermal Thiele modulus and activation energy parameters. Using the Matlab / Scilab program, we also derive the numerical solution to this problem. Simulated data and previously published limiting cases are used to validate the new analytical results. A reasonable agreement is observed.

Keywords: self-igniting, Gas reactant, temperature, Thiele modulus, activation energy, mathematical modelling
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1 Introduction

The self-combustion of coal heaps in the absence of natural convection has been studied by Continillo et. al. in [10] and [11]. Convection, reaction, and diffusion are the three key factors in the coal stock piles; ability to self-ignite. The observation of steady regimes results from a thorough numerical modelling of coal stockpiles that automatically ignite. Two streamlined distributed-parameter models that include heat conduction, mass diffusion, and a one-step Arrhenius exothermic chemical reaction were explored in order to better understand this phenomenon. With simple finite-difference techniques, both model equations were solved [12]. On the other hand, Continillo et al. [13] studied the dynamic behavior of at two-dimensional coal pile also by accounting for natural convection. As part of a comprehensive study of self-heating of coal stockpiles, a simple mathematical model has been developed. A spontaneous combustion

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reaction occurs in a bed of solid fuel, and flow is caused by natural convection caused by the onset of temperature gradients within the pile. This problem of spontaneous ignition of coal stockpiles is challenging due to the safety implications and its theoretical complexity. When coal reacts with atmospheric oxygen to produce heat that is not effectively evacuated to the outside ambient, coal stockpiles self-ignite [16]. The analysis is conducted in a twofold way. From one side, we characterise the model predictions with a parameter-continuation tool. This approach is capable of describing most of the details of the bifurcation structure of the model, but some complex situations are not captured. Therefore, a simulative analysis is conducted to characterise these exotic dynamics. As it will be shown, also mixed-mode oscillations can arise [9].

Mathematical models that emerge from modern complex nonlinear reaction diffusion systems for which exact solutions can't be found, and therefore researchers are opting for approximate numerical or analytical solutions. Though numerical solutions are relatively easy to obtain, some of their shortcomings cannot be avoided. In particular, the stability of the approximate numerical solution is not always guaranteed. In addition, with numerical solutions, it is difficult to adjust the model parameters to mimic the numerical data. With modern computational tools, many reliable and highly accurate analytical methods, which have been established in recent years, can be used to solve the underlying nonlinear system of the most common method that has shown remarkable success in solving complex nonlinear systems. These methods include the variation iteration method [1], homotopy analysis method [20], differential transformation method [8], Green's function-fixed point method [3], [4], [2], exp-function method [18], and Taylor series method [17], [19] and [22]. Using this concept, Felicia et al [15] have previously obtained the semi analytical solution for the self igniting system using the Modified Adomain Decomposition method. Ananthswamy et al. [6] have derived semi analytical using Homotopuy perturbation method for self igniting system only for small values of Thiele modulus and heat of reaction and activation energy. This article employs Akbari-Ganji's method [5], which is highly accurate, efficient, and widely accessible to scientists other than mathematicians.

As discussed above, researchers have employed several analytical approaches for self igniting only numerical analysis and semi analytical analysis. To the best of our knowledge,there is no concise and closed-form analytical equation provided for concentration of gas reactant and temperature. This study intends to obtain new analytical expressions, in closed form, for the concentration of the gas reactant and temperature for experimental values of heat of reaction, thermal Thiele modulus and activation energy parameters.

2 Mathematical analysis of the problem

We discuss the issue of self-ignition in a reaction diffusion system in this study. The governing equations are those of a dynamic model with distributed parameters for heterogeneous reaction in a one-dimensional layer. Through the reaction media, the gaseous reactant diffuses. An exothermic chemical reaction of first order occurs in one step. Through the conventional Arrhenius exponential, the reaction rate is temperature dependent. One mass balance equation for the gas reactant is constructed since consumption of the solid reactant is disregarded. Gas and solid temperature are equal, thus, only one energy balance equation is written. This equation accounts for heat conduction, and contains a source term due to the reaction. The steady state governing equation are given by [9]

$$\frac{\partial Y}{\partial t} = L_e \frac{\partial^2 Y}{\partial x^2} - \phi^2 Y \exp(-\frac{\gamma}{T}) \tag{2.1}$$

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \beta\phi^2 Y \exp(-\frac{\gamma}{T}), \tag{2.2}$$

where Y is the concentration of the gas reactant, T is the temperature, x is the spatial co-ordinates¸ L_e (the Lewis number) is the ratio between mass and heat diffusivities, the parameter β is a dimensionless heat of reaction, the parameter ϕ^2 is the thermal Thiele modulus, and γ is a dimensionless activation energy (refer to notation for more details). The boundary conditions are

$$T(0,t) = T(1,t) = 1, Y(0,t) = 1, \frac{\partial Y}{\partial x}|_{x=1} = 0 \text{ for } t > 0.$$

Under steady state condition, equations (2.1) and (2.2) becomes

$$\frac{d^2 Y}{dx^2} - \frac{\phi^2}{L_e} Y \exp(-\frac{\gamma}{T}) = 0, \tag{2.3}$$

$$\frac{d^2 T}{dx^2} + \beta\phi^2 Y \exp(-\frac{\gamma}{T}) = 0 \tag{2.4}$$

with boundary conditions

$$T = 1, Y = 1, \text{ at } x = 0 \tag{2.5}$$

$$T = 1, \frac{dY}{dx} = 0, \text{ at } x = 1. \tag{2.6}$$

3 Analytical expression of the concentration of gas reactant and temperature using Akbari Ganji method

The Akbari-Ganji method (AGM), which was first put forth by M. Akbari and D. Ganji has been successfully applied to find analytical solutions of nonlinear systems. Berkan et al. [7] investigated the 3D problem of condensation film on inclined rotating disk electrodes analytically using AGM. Derakhshan et al. [14] used AGM to discuss the process of heat and mass transfer in steady nano-fluid flow between two parallel plates in the existence of a uniform magnetic field. Saravanakumar et al. [21] employed the AGM to solve a nonlinear reaction-diffusion equation in an immobilized enzymes system There are no accurate solutions to the nonlinear systems (2.3)-(2.6). In terms of the features of the controlling system, it was also suggested that approximate analytical approaches, rather than numerical ones, are more valuable. Using Akbari-Ganji method, we achieve highly accurate and reliable approximation analytical results in this part.The approximate solution for the concentration of the gas reactant and temperature is as follows [Appendix A]:

$$Y(x) = \frac{\cosh(\alpha(x-1))}{\cosh(\alpha)} \tag{3.1}$$

$$T(x) = \frac{\sinh(\delta(1-x))}{\sinh(\delta)} + \frac{\sinh(\delta x)}{\sinh(\delta)}. \tag{3.2}$$

The unknown constant "δ and α" are obtained using the following equations.

$$\alpha = \sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}} \tag{3.3}$$

$$\delta = \sqrt{-\beta\phi^2 e^{-\gamma}}. \tag{3.4}$$

4 Numerical Simulation

The function pdex4 in SCILAB software, which solves the boundary value problems for differential equations, is used to solve equations (2.3)-(2.6). Upon comparison in the figures 1-2, it is evident that both the results give satisfactory agreement. In Tables (2-4) and Figures 1 and 2, the analytical results for the concentration of the gas reactant and temperature in the self-igniting reaction diffusion system were compared to simulation data and previously available analytical results (ADM) and (HPM). The maximum average error between our new analytical result (AGM method) and simulation result is 0.003% in gas reactant and 0% in temperature. But the previous analytical result (ADM and HPM method) has a maximum average error of 45% in gas reactant and 18% in temperature.

5 Results and Discussion

To assess the accuracy of the AGM solution with a finite number of terms, the system of differential equations was numerically solved. Our analytical data are graphically compared with numerical result to demonstrate the efficacy of the present method. Equations (2.3)-(2.6) give a simple and innovative analytical expression of concentration of gas reactant and temperature in the self igniting reaction diffusion system, respectively. From the figure1-2, it is evident that as thermal thiele modulus ϕ increases Y decreases and as activation energy γ increases gas reactant Y also increases. Further as thermal thiele modulus ϕ increases temperature T also increases while as activation energy γ increases temperature T decreases. Concentration of gas reactant and temperature are affected by the parameters ϕ^2 and β . The Thiele modulus ϕ^2 can be varied by altering the torus doubling sequences and of period-adding bifurcation sequences. The parameter β is affected by the temperature as well as the thermal Thiele modulus and activation energy parameters.

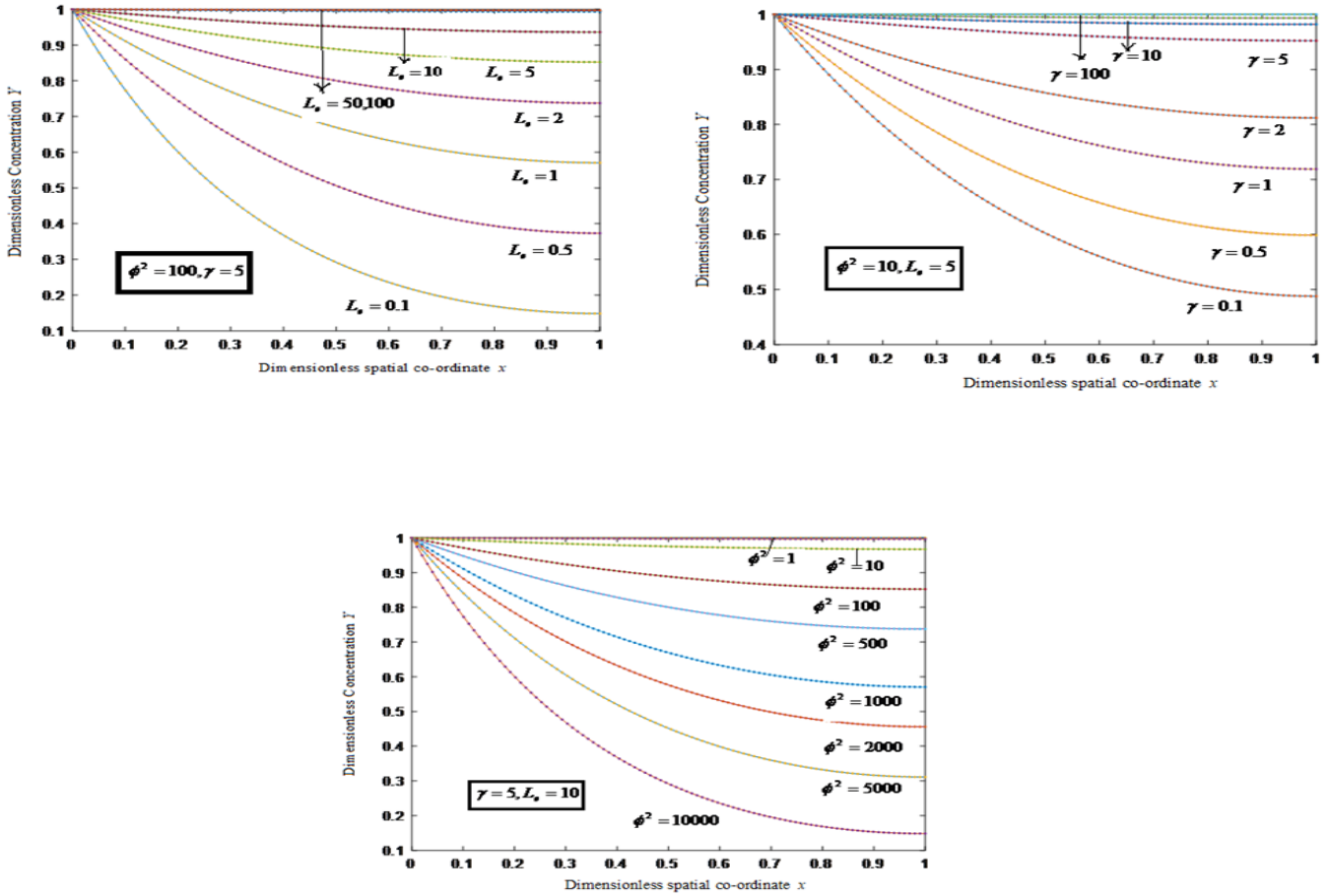

Figure 1: Comparison Analysis of Akbari Ganji method are in solid agreement with the numerical results obtained by Maple RK45 procedure (Fehlberg fourth-fifth order Runge-Kutta method with degree four interpolant) for various values of the experimental parameters [6].

6 Conclusion

This paper gives a detailed theoretical analysis of self igniting reaction diffusion system using modelling. A non-linear time-independent differential equation has been solved using the Akbari-Ganji method. Approximate analytical expressions for the concentration of gas reactant and temperature have been derived. These derived approximate analytic results concurred with MATLAB-generated numerical results. Moreover, the simplicity and reliability of the proposed approaches, as well as their accessibility, would make them usable for determining the approximate amounts of gas reactant and temperature. The concentrations were approximated using this method for the first time. The resultant approximation expressions of the concentration were highly accurate compared to this multiplicity of dynamic steady states has different and new characteristics with respect to the sequence of alternating mixed-mode oscillations and chaos often reported in the literature for chemical reactors.

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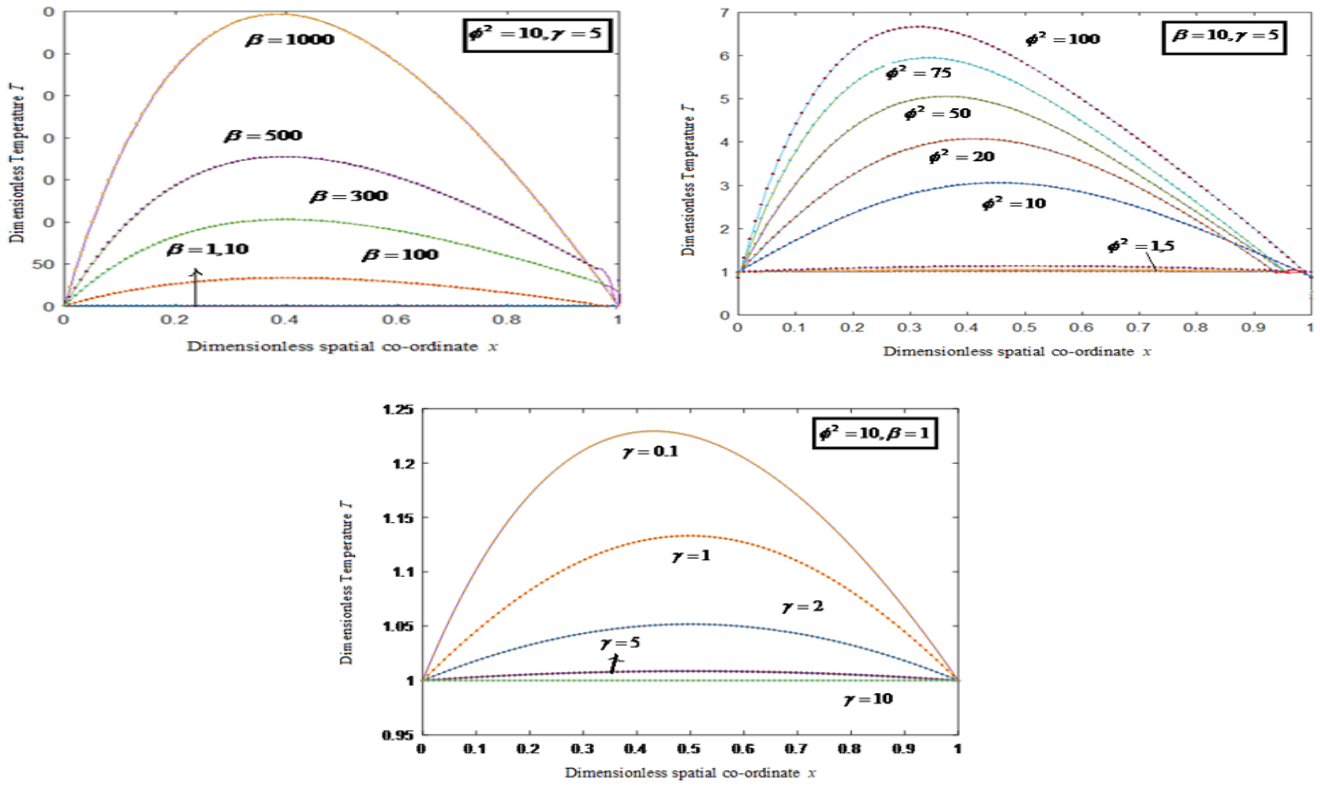

Figure 2: Comparison Analysis of Akbari Ganji method are in solid agreement with the numerical results obtained by Maple RK45 procedure (Fehlberg fourth-fifth order Runge-Kutta method with degree four interpolant) for various values of the experimental parameters [6].

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Appendix A

The solution of equations (2.3)-(2.6) is using Akbari Ganji method The approximate analytical solutions for the equation (2.3) and (2.4) are considered as follows:

$$u(x) = A_1\cos(\alpha x) + B_1\sin(\alpha x) \tag{A.1}$$
$$v(x) = A_2\cos(\delta x) + B_2\sin(\delta x) \tag{A.2}$$

Using the boundary conditions (2.5) and (2.6), the constants becomes $A_1 = 1, B_1 = -\tanh\alpha$ and $A_2 = 1, B_2 = \frac{1-\cosh(\delta)}{\sinh(\delta)}$. Then the equations (A.1) and (A.2) becomes

$$Y(x) = \frac{\cosh(\alpha(x-1))}{\cosh\alpha} \tag{A.3}$$
$$T(x) = \frac{\sinh(\delta(1-x))}{\sinh(\delta)} + \frac{\sinh(\delta x)}{\sinh(\delta)} \tag{A.4}$$

The unknown constant δ and α are obtained using the following equations. Substituting Eqs. (A.3) and (A.4) in (2.3) & (2.4), we get

$$\frac{\alpha^2\cosh(\alpha(x-1))}{\cos(\alpha)} - \frac{\phi^2}{L_e}\frac{\cosh(\alpha(x-1))}{\cos(\alpha)}\exp\left(\frac{-\gamma}{\frac{\sinh(\delta(1-x))}{\sinh(\delta)} + \frac{\sinh(\delta x)}{\sinh(\delta)}}\right), \tag{A.5}$$

$$\frac{\delta^2\sinh(\delta(1-x))}{\sinh(\delta)} + \frac{\delta^2\sinh(\delta x)}{\sinh(\delta)} + \beta\phi^2\frac{\cosh(\alpha(x-1))}{\cosh(\alpha)}\exp\left(\frac{-\gamma}{\frac{\sinh(\delta(1-x))}{\sinh(\delta)} + \frac{\sinh(\delta x)}{\sinh(\delta)}}\right). \tag{A.6}$$

Solving (A.5) and (A.6), we get the values of δ and α.

$$\alpha = \sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}} \tag{A.7}$$
$$\delta = \sqrt{-\beta\phi^2 e^{-\gamma}}. \tag{A.8}$$

Appendix B

MATLAB Code for Numerical Solution of the Non-linear equations (2.3)**-**(2.6)

```
function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,1000000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
figure
plot(x,u1(end,:))
title('u1(x,t)')
```

```
xlabel('Distance x')
ylabel('u1(x,2)')
figure
plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
ylabel('u2(x,2)')
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1; 1] .* DuDx;
l = 10;
p =100;
b =1;
g =10;
F = -p*u(1)*exp(-g/u(2))/l;
F1 = b*p*u(1)*exp(-g/u(2));
s=[F; F1];
function u0 = pdex4ic(x);
u0 = [1; 1];
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = [ul(1)-1; ul(2)-1];
ql = [0; 0];
pr = [0;ur(2)-1];
qr = [1; 0];
```

Table 1: Nomenclature

S. No	Symbol	Description
1.	c_0	Concentration of the free stream
2.	c_p	Specific heat
3.	D	Mass diffusivity
4.	E	Activation energy
5.	K_0	Pre exponential factor
6.	L	Layer thickness
7.	L_e	Lewis number, (D/α)
8.	R	Gas reactant
9.	T	Dimensionless temperature $(\bar{T}/\bar{T_0})$
10.	$\bar{T}$	Temperature
11.	$\bar{T_0}$	Free stream temperature
12.	t	Dimensionless time $\bar{t}\alpha/L^2$
13.	$\bar{t}$	Time
14.	Y	Dimensionless concentration c/c_0
		Greek Letters
15.	α	Thermal diffusivity
16.	β	Dimensionless heat reaction $\left(-\Delta H c_0/\rho c_p \bar{T_0}\right)$
17.	γ	Dimensionless activation energy $E/R\bar{T_0}$
18.	ΔH	Enthalpy of reaction
19.	ρ	Density
20.	ϕ	Thiele number, $\sqrt{k_0 L^2/\alpha}$

Table 2: Various approximate analytical expression concentrations of gas reactant and temperature

Felicia work [6] limiting cases		
S. No.	Concentration of the gas reactant	Concentration of the temperature
1.	$Y(x) = 1 + \frac{\phi^2}{L_e}e^{-\gamma}\left(\frac{x^2}{2} - x\right) + \frac{\phi^4}{L_e}e^{-2\gamma}$ $\left[\frac{1}{L_e}\left(\frac{x^4}{24} - \frac{x^3}{6} + \frac{x}{3}\right) - \frac{\gamma\beta}{2}\left(\frac{x^4}{12} - \frac{x^3}{6} + \frac{x}{6}\right)\right]$	$T(x) = 1 - \beta\phi^2 e^{-\gamma}\left(\frac{x^2}{2} - \frac{x}{2}\right) -$ $\beta\phi^4 e^{-2\gamma}\left[\frac{1}{L_e}\left(\frac{x^4}{24} - \frac{x^3}{6} + \frac{x}{8}\right) - \frac{\gamma\beta}{2}\left(\frac{x^4}{12} - \frac{x^3}{6} + \frac{x}{12}\right)\right]$
Ananthaswamy et al. [5] limiting cases		
2.	$Y(x) = \frac{[e^{2(x-1)}\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}+1]e^{(2-x)\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}}}{e^2\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}+1}$	$T(x) = -\frac{1}{e^2\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}+1}e^{-(x-1)}\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}+1}\Big[\beta L_e e^{(2x-1)\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}}$ $+(-1+L_e(x-1)\beta)e^{(x-1)\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}}+(-1+\frac{\phi^2 e^{-\gamma}}{L_e})L_e(x-1)\beta)$ $\times e^{(x-1)\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}} + (-1+L_e(x-1)\beta e^{(1+x)\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}})$ $-2L_e\beta\Big(xe^{\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}x} - \frac{e^{\sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}}}{2}\Big)\Big]$
This work all values of parameters		
3.	$\frac{\cosh(\alpha(x-1))}{\cosh(\alpha)}$, where $\alpha = \sqrt{\frac{\phi^2 e^{-\gamma}}{L_e}}$	$\frac{\sinh(\delta(1-x))+\sinh(\delta x)}{\sinh(\beta)}$, where $\delta = \sqrt{-\beta\phi^2 e^{-\gamma}}$

Table 3: Comparison of Analytical result with numerical result and various analytical results for concentration of gas reactant $Y(x)$ for various of parameter $L_e = 10, \gamma = 5, \beta = 1$

Case I: $\phi^2 = 100$

x	Numerical Simulation	This work	Rajendran et al. [5]	Anathaswamy et al. [6]	Error for this work	Error for Rajendran et al. [5]	Error for Anathaswamy et al. [6]
0	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
0.2	0.9881	0.9881	0.9844	0.9845	0.0000	0.3745	0.3643
0.4	0.9788	0.9788	0.9722	0.9721	0.0000	0.6743	0.6845
0.6	0.9723	0.9723	0.9638	0.9639	0.0000	0.8742	0.8639
0.8	0.9685	0.9684	0.9591	0.9590	0.0103	0.9706	0.9809
1.0	0.9673	0.9672	0.9578	0.9579	0.0103	0.9821	0.9718
Average Error					0.0034	0.6459	0.6442

Case II: $\phi^2 = 1000$

x	Numerical Simulation	This work	Rajendran et al. [5]	Anathaswamy et al. [6]	Error for this work	Error for Rajendran et al. [5]	Error for Anathaswamy et al. [6]
0	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
0.2	0.9012	0.9012	0.5395	0.5395	0.0000	40.1354	40.1353
0.4	0.8273	0.8273	0.4747	0.4747	0.0000	42.6206	42.6205
0.6	0.7763	0.7762	0.3602	0.3602	0.0128	53.6004	53.6004
0.8	0.7466	0.7465	0.2678	0.2678	0.0134	64.1307	64.1307
1.0	0.7378	0.7373	0.1881	0.1881	0.0677	74.5052	74.5053
Average Error					0.0156	45.8320	45.8320

Table 4: Comparison of Analytical result with numerical result and various analytical results for temperature $T(x)$ for various of parameter $\phi^2 = 100, \gamma = 5, L_e = 1$

Case I: $\beta = 10$

x	Numerical Simulation	This work	Rajendran et al. [5]	Anathaswamy et al. [6]	Error for this work	Error for Rajendran et al. [5]	Error for Anathaswamy et al. [6]
0	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
0.2	2.3010	2.3010	2.8345	2.8340	0.0000	23.1855	23.1638
0.4	3.4980	3.4980	4.4132	4.4135	0.0000	26.1635	26.1720
0.6	3.5460	3.5460	4.3410	4.3411	0.0000	22.4196	22.4224
0.8	2.6920	2.6920	3.3289	3.3289	0.0000	0.0000	0.0000
1.0	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
Average Error					0.0000	15.9046	15.9028

Case II: $\beta = 5$

x	Numerical Simulation	This work	Rajendran et al. [5]	Anathaswamy et al. [6]	Error for this work	Error for Rajendran et al. [5]	Error for Anathaswamy et al. [6]
0	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
0.2	1.4131	1.4130	1.6512	1.6510	0.0070	16.8494	16.8353
0.4	1.5921	1.5921	2.1131	2.1131	0.0000	32.7240	32.7240
0.6	1.6132	1.6132	2.2521	2.2522	0.0000	39.7240	32.7240
0.8	1.4155	1.4156	1.7321	1.7320	0.0070	22.3666	22.3595
1.0	1.0000	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
Average Error					1.99976E-06	18.5907	18.5882