Journal of Mathematics and Statistics 3 (4): 233-236, 2007
ISSN 1549-3644

Numerical Solution For Frank-Kamenetskii And Activation Energy Parameters in Reactive-Diffusive Equation with Variable One-Exponential Factor

[1]O.K. Koriko and [2]A.J. Omowaye
[1]Department of Mathematical Sciences, Federal University of Technology,
P.M.B 704, Akure, Ondo State
[2]Department of Mathematical Sciences, University of Ado-Ekiti,
P.M.B 5363, Ado-Ekiti, Ekiti State

Abstract: In this study, we considered a steady state, exothermic chemical reaction, taking the diffusion of the reactant into account and assuming an Arrhenius temperature dependence with variable pre-exponent factor. Numerical solution is constructed for the governing nonlinear boundary value problem using finite difference scheme .The effect of Frank-Kamenetskii, activation energy parameter and pre-exponent factor on the temperature were also examined, result were displayed in graphs.

Key words: Numerical solution, arrhenius kinetics, pre-exponent factor, existence and uniqueness, exothermic

INTRODUCTION

Enring[3] described a Swedish chemist, Svante Arrhenius as the developer of an important equation which shows that there is an exponential relationship between rate constant of a chemical reaction and temperature. According to him, Arrehenius (1889), gave the equation as:

$$K = Ae^{-\frac{Ea}{RT}}$$

Where:

K = The rate constant
R = The gas constant known as Boltzman gas constant
T = The temperature in degree Kelvin.

A is a constant known as Arrhenius constant which Walas[12] described as the pre-exponential factor while Ramsdem[11] described the same constant A as the rate of collision between the molecules. Also, he described the activation energy Ea as the energy which the colliding molecules must possesses before a collision will result in reaction. Furthermore, the theory of nonlinear reaction diffusion equations is quite elaborate and their solution in rectangular, cylindrical and spherical coordinate remains an extremely important problem of practical relevance in the engineering sciences[1,7]. Makinde[6] reported that the improvement in thermal systems as well as energy utilization during the convection in any fluid is one of the fundamental problems of the engineering processes, since improved thermal systems will provide better material processing, energy conservation and environmental effects. It must also be remarked here that understanding of the factors that control the thermal ignition of combustible materials consisting of the mathematical equations (1) and (2) is of fundamental importance in many industrial processes (Bowes[3] for some special cases). Makinde[8] examined the steady-state solutions of a strongly exothermic reaction of a viscous combustible material in a channel filled with a saturated porous medium under Arrhenius kinetics neglecting reactant consumption. He modelled the problem by employed the Brinkman model and constructed analytical solutions for the governing nonlinear boundary value problem using a perturbation technique together with a special type of Hermite-pade approximants and important properties of the temperature field including bifurcations and thermal critically were discussed. Okoya[9] reported similarity temperature profiles for some nonlinear reaction-diffusion equations and investigated two models: one is power law dependence and the other is exponential dependence. In both cases, he assumed a heat source term with spatial polynomial delay is known to have been applied earlier under some physically reasonable assumptions. In particular, the

Corresponding Author: Dr. O.K. Koriko, Department of Mathematical Sciences, Federal University of Technology Akure, P.M.B. 704, Akure, Ondo State, Nigeria

solutions obtained permit us to compare the contribution of the heat source term and geometry. Finally, a realistic mathematical description of thermal explosion needs to include the effects of Arrhenius temperature dependence with variable pre-exponential factor (Ayeni[1], Dainton[4]).

In this present study, special attention has been given to the combined effects of Frank-Kamenetskii, activation energy parameters and pre-exponent factor on the temperature rise of the system. We must remark that Okoya[10] studied the case of r(-2,0) but we are taking our r to be 0.5 which is the case of bimolecular reaction. In the following sections the problem is formulated, analysed, solved and discussed.

MATHEMATICAL MODEL

We consider the steady-state, exothermic chemical reaction, taking the diffusion of the reactant in a slab into account and assuming an Arrhenius temperature dependence with variable pre-exponential factor. The equation for the temperature T(x) of a one-dimensional slab, with boundaries lying in the co-ordinate planes $x = \pm\alpha$, may be written in terms of physical variables, following[10]:

$$\lambda \frac{d^2T}{dx^2} + \rho^{QA}\left(\frac{KT}{xh\rho}\right)^r \exp\left(-\frac{E}{RT}\right) = 0 \qquad (1)$$

The appropriate boundary conditions are

$$T = T_0 \quad \text{on} \quad x = \pm\alpha \qquad (2)$$

Where:

λ = The thermal conductivity of the material
Q = The heat of reaction A is the rate constant
ν = The vibration frequency
K = The planck's constant ρ is the density
R = The densiy, R is the universal gas constant
E = The activation energy r is the exponent
T_o = The initial temperature

The following dimensionless variables and parameters are introduced:

$$\bar{x} = \frac{x}{a}, \theta = \frac{T - T_0}{E/RT_0^2} \text{ and } \varepsilon = RT_o/E \qquad (3)$$

Neglecting the bar symbol for clarity, the dimensionless governing equations are obtained as:

$$\frac{d^2\theta}{dx^2} + \delta(1+\varepsilon\theta)^r \exp\left(\frac{\theta}{1+\varepsilon\theta}\right) = 0 \qquad (4)$$

Where,

$$\delta = a^2 QEA(KT_0/\nu h\rho)^r \exp(-E/RT_o)/\lambda RT_o^2$$

is the Frank-Kamenetskii parameter, $\varepsilon = RT_o/E$ is the activation energy parameter.

Bowes[3], Dainton[4] reported that it has been shown experimentally that this model is able to predict the critical ignition temperature for a variety of combustible materials while Ayeni[2] studied an asymptotic analysis of a spatially homogeneous model of a non-isothermal branched-chain reaction ,in particular he showed the explosion time and provide an upper bound for it as a function of the activation energy which can vary over all positive value.

EXISTENCE OF UNIQUE SOLUTION

In this section we shall show that there exists a unique solution of (4):

Let

$$D\{x,\theta): -1 \le x \le 1 \text{ and } 0 \le \theta \le R\} \text{ and}$$
$$P = \{0 < \delta \le T, 0 < r \le u\}$$

$$D\{x,\theta): -1 \le x \le 1 \text{ and } 0 \le \theta \le R\} \text{ and}$$
$$P = \{0 < \delta \le T, 0 < r \le u\}$$

Theorem: Let D and P hold where R, T, U and real constants, then for $\varepsilon > 0$ there exist a unique solution of problem (4, 5).

Proof: The boundary value problem (4,5) is reduced to initial value problems with the initial conditions

$$\theta(-1) = 0 \text{ and } \frac{d\theta(-1)}{dx} = \alpha$$

Where α is a guess value that satisfies $\theta(1) = 0$

$$y_1 = x, y_2 = \theta, y_3 = \theta^1$$

Let
Then

$$\left.\begin{aligned} y_1^1 &= 1 \\ y_2^1 &= \theta^1 \\ y_3^1 &= \theta^{11} \end{aligned}\right\} \qquad (6)$$

The relation in (6) can be represented as

$$\begin{pmatrix} y_1^1 \\ y_2^1 \\ y_3^1 \end{pmatrix} = \begin{pmatrix} 1 \\ y_3 \\ -\delta(1+\varepsilon\theta)^r \exp\left(\dfrac{\theta}{1+\varepsilon\theta}\right) \end{pmatrix} \tag{7}$$

satisfying the initial condition

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ \alpha \end{pmatrix} \tag{8}$$

Equations 7 and 8 is equivalently written as:

$$y^1 = f(y_1, y_2, y_3),\ y(-1) = y_0$$

That is

$$\begin{pmatrix} y_1^1 \\ y_2^1 \\ y_3^1 \end{pmatrix} = \begin{pmatrix} f_1(y_1, y_2, y_3) \\ f_2(y_1, y_2, y_3) \\ f_3(y_1, y_2, y_3) \end{pmatrix} \tag{9}$$

Thus,

$\dfrac{\partial f_i}{\partial y_j}, i, j = 1,2,3$ is bounded and there exist K (where K = max (k_{ij}) such that

$$\left|\frac{\partial f_i}{\partial y_j}\right| \le K \quad \text{where } 0 < K < \infty$$

Therefore, $f_i(y_1, y_2, y_3)$, i = 1,2,3 are Lipschitz continuous. Hence there exist a unique solution of (4,5).

METHOD OF SOLUTION

Due to the nonlinear nature of the governing Eq. 4, 5, it is convenient to solve the equation by the use of the finite difference scheme. A system of rectangular grids was used for the application of the difference scheme over the triangular domain. Using computer symbolic algebra package MAPLE (F solve) the equation can easily be handled and the result is presented below.

RESULT AND DISCUSSION

The behaviour of solutions for the nonlinear reaction diffusion equations with variable pre-exponential factor can be summarized as follows:

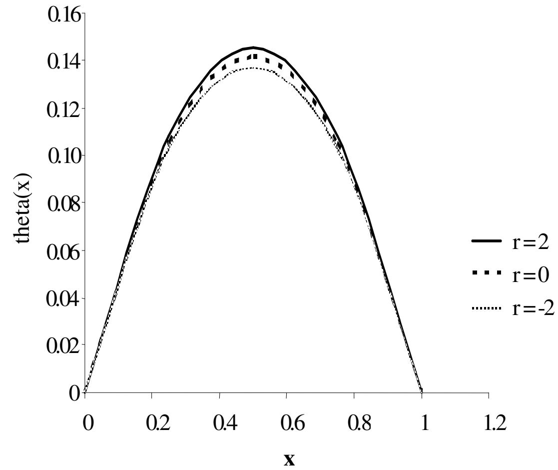

Fig. 1: The graph of theta(x) against x for various value of r and for fixed value of ε = 1

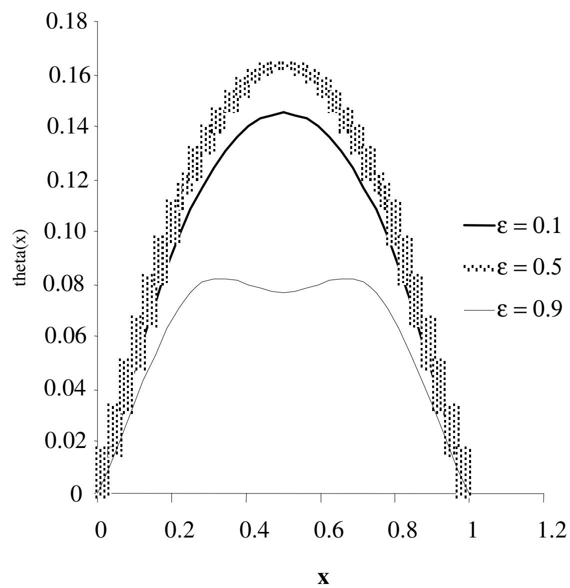

Fig. 2: The graph of theta ε (x) against x for various value of and fixed value of r

Simple model for non linear reaction-diffusion equation with variable pre-exponential factor has been developed. Also, the existence and the uniqueness theorem for the resulting second order differential equation has been presented. The important parameter in the problem is δ, ε which is a reflection of the internal properties of the given system. Finally, the numerical solution is also given.

Figure 1 shows the graph of temperature θ(x) against position x for ε = 0.1, δ = 1 and various values

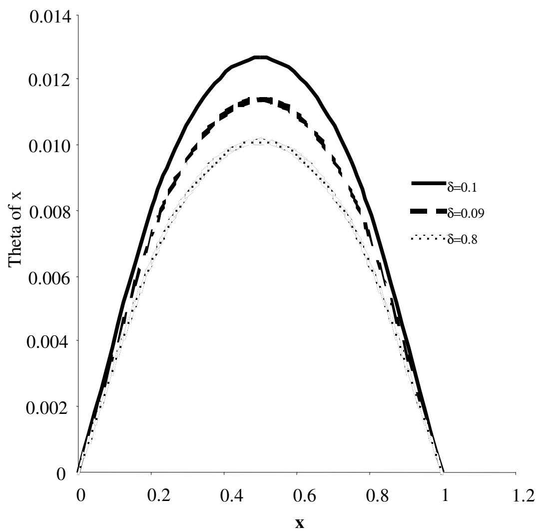

Fig 3: The graph of theta of x against position x for various values of and for fixed valued of

of r = (2, 0, -2) ,the graph is parabolic and reveals that the temperature increases as the value of r increases, this maximum temperature occurs at θ(x) = 0.1453100080. We also remarked that the problem is not admissible for r = 0.5 or r = -0.5. Figure 2 shows the graph of temperature θ(x) against position x for r = 2, δ = 1 and for various values of ε = (0.1,0.5,0.9), it is observed that the temperature of the medium fluctuates for various value of ε, for ε = 0.1 the maximum temperature θ(x) is 0.1453100080 while for ε = 0.5 the maximum temperature θ is 0.1639913398, for ε = 0.9 the maximum temperature θ is 0.07674921513. Figure 3 shows the graph of θ(x) against position x for various values of δ =(0.1, 0.09, 0.08) and fixed valued of r=2, ε = 0.1. It is observed that as δ decreases the temperature of the medium decreases.

CONCLUSION

Reactive-diffusive equation with variable pre-exponential factor for one-step Arrhenius reactions was examined. The existence and uniqueness of solution was established, while results were also displayed in graphs.

REFERENCES

1. Al-Hadhrami, A.K., L. Elliot and D.B. Ignham, 2003 A new model for viscous dissipation in porous media across a range of permeability values. Transp. Porous Media, 53:117-122.
2. Ayeni, R.O., 1982. On the explosion of chain-thermal reaction. J. Aust. Math. Soc. Series, 24: 194-202
3. Bowes, P.C., 1984. Self-Heating: Evaluating and Controlling the Hazard. Elsevier, Armsterdam.
4. Dainton, F.S., 1960. Chain Reaction: An introduction Wiley, New York.
5. Enring, H., 1990. The Encyclopedia: Am. Grolier Incorporated, 2: 377.
6. Makinde, O.D., 2004. Exothermic explosions in a slab: A case study of series summation technique. Int. Comm. Heat Mass Transfer., 31: 1227.
7. Makinde, O.D., 2005. Strong Exothermic explosions in a cylindrical pipe: A case study of series summation technique. Mech. Res. Comm., 32: 191-195.
8. Makinde, O.D., 2006. Thermal ignition in a reactive viscous flow through a channel tilled with a porous medium. A.S.M.E. J. Heat Transfer, 128: 601-604.
9. Okoya, S.S., 2001. Similarity temperature profiles for some nonlinear reaction-diffusion equations. MEch. Res. Comm., 28: 477-484.
10. Okoya, S.S., 2004. Reactive-diffusive equation with variable pre-exponential factor. Mech. Res. Comm., 31: 263-267.
11. Ramsden, E.N., 1990. A level chemistry (3rd Edn) Stanley Thornes Ltd., Cheltenham.
12. Wala, M., 1969. Perry's Chemical Engineers' Handbook McGraw-Hill Companies Incorporated, USA.