

Temperature profile of two steps Arrhenius, Bimolecular and Sensitized exothermic chemical reactions in a slab

^a P. O. Olanrewaju, ^b A.S. Bishop and ^c O.T. Arulogun

^aDepartment of Pure and Applied Mathematics

^cDepartment of Computer Science and Engineering

Ladoke Akintola University of Technology, Ogbomosho, Nigeria

^bDepartment of Mathematics, Covenant University, Ota.

Abstract

In this study, we examine the unsteady state of a two step exothermic chemical reaction in a slab, taking the diffusion of the reactant into account and assuming a temperature dependent pre-exponential factor. The nonlinear partial differential equation governing the transient reaction-diffusion problem is solved numerically using a semi-discretization finite difference technique. We observed that the maximum temperature is obtained in bimolecular type of reaction. It was established that the steady state solution was reached at $t = 0.5$ which allow us to see the influence of other parameters coming into the model.

Keywords: Temperature profile; Two steps exothermic reaction; Thermal stability; bimolecular; sensitized; Arrhenius; slab

Nomenclature

T	absolute temperature,	T_0	initial temperature,
T_w	wall temperature,	\bar{t}	time,
k	thermal conductivity	Q_1	first step heat of reaction
Q_2	second step heat of reaction	A_1	first step reaction rate
A_2	second step reaction rate	E_1	first step activation energy
E_2	second step activation energy,	R	universal gas constant,
C_2	second step initial concentration	h	Planck's number
K	Boltzmann's constant	a	slab half width,
\bar{y}	normal coordinate	c_p	specific heat at constant pressure
m	numerical exponent	r	activation energy ratio parameter
b	slab initial temperature		

Greek symbols

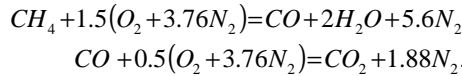
λ	Frank-Kamenetskii parameter
λ_c	critical parameter
ε	activation energy parameter
β	two step reaction parameter
θ	dimensionless temperature
ρ	density,
ν	vibration frequency

1.0 Introduction

Some combustion research problems have been considered as fluid mechanism problems that include heat release by chemical reactions. Accordingly, It was observed in [1] that this was useful to some extent for designing stationary combustion processes but was not sufficient for ignition, quenching or pollutant cases, thus, the coupling of large reaction mechanism, fluid flow and combustion; of fluid mechanism of turbulent flow with density change by heat release is necessary for the treating of ignition and quenching. In nature, and particularly in industry, rapid exothermic reaction processes which take place with the evolution of large amounts of heat are considerably important. Such processes have long been called combustion processes. Thermal runaway is one of the most interesting topics in the study of nonlinear partial differential equations arising in combustion theory [2]. Many authors have investigated several idealized problems of

^aCorresponding author: E-mail oladapo_anu@yahoo.ie , Tel. +23481385550

combustion in a chemically reacting flow system as a one step reaction model [3-7]. Although this assumption may be true for some problems, however, in most combustion processes a single reaction step is not sufficient to describe flame propagation [8-9]. Similarly, the combustion taking place within k-fluid is treated as a two step irreversible chemical reaction of methane oxidation as follows [10-14]:



Our purpose here is to determine when the unsteady equation reach a steady state (i.e. the value of t that will make the solution reach a steady state). It is an extension of Olanrewaju [14].

2.0 Mathematical Formulation

We consider a two step exothermic chemical reaction of combustible materials in a slab, taking into account the diffusion of the reactant and the temperature dependent variable pre-exponential factor (see Fig. 1).

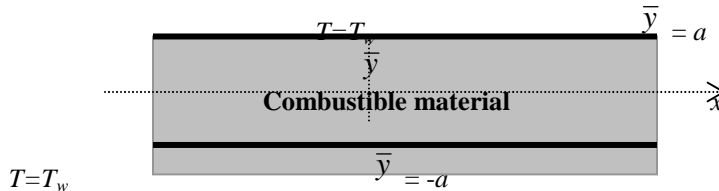


Fig. 1. Sketch of the physical model.

Following [2, 8, 9, 11], the equation for the heat balance in the original variables can be written as

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial \bar{y}^2} + Q_1 C_1 A_1 \left(\frac{KT}{vh} \right)^m e^{-\frac{E_1}{RT}} + Q_2 C_2 A_2 \left(\frac{KT}{vh} \right)^m e^{-\frac{E_2}{RT}} = 0, \quad (2.1)$$

with the initial and boundary conditions given as

$$T(\bar{y}, 0) = T_0, \quad (2.2)$$

$$\frac{\partial T}{\partial \bar{y}}(0, \bar{t}) = 0, T(a, \bar{t}) = T_w \text{ for } \bar{t} > 0, \quad (2.3)$$

where T is the absolute temperature, T_0 is the initial temperature, T_w is the wall temperature, \bar{t} is the time, k is the thermal conductivity of the material, Q_1 and Q_2 are the heats of reaction in the first and second step, A_1 and A_2 are the reaction rate constants in the first and second step, E_1 and E_2 are the activation energies in the first and second step, ρ is the density, R is the universal gas constant, C_1 and C_2 are the initial concentration of the reactant species in the first and second step, h is the Planck's number, K is the Boltzmann's constant, v is vibration frequency, a is the slab half width, \bar{y} is distance measured in the normal direction to the plane c_p is the specific heat at constant pressure and m is the numerical exponent such that $m = \{-2, 0, \frac{1}{2}\}$ represent numerical exponent for Sensitised, Arrhenius and Bimolecular kinetics respectively ([8]). The following dimensionless variables are introduced into Eqs. (2.1)-(2.3):

$$\theta = \frac{E_1(T - T_w)}{RT_w^2}, \quad \varepsilon = \frac{RT_w}{E_1}, \quad y = \frac{\bar{y}}{a}, \quad \beta = \frac{Q_2 C_2 A_2}{Q_1 C_1 A_1} e^{-\frac{E_1 - E_2}{RT_w}}, \quad r = \frac{E_2}{E_1}, \quad (2.4)$$

$$\lambda = \frac{E_1 a^2 Q_1 C_1 A_1}{k R T_w^2} \left[\frac{K T_w}{v h} \right]^m e^{-\frac{E_1}{R T_w}}, \quad t = \frac{k \bar{t}}{\rho c_p a^2}, \quad b = \frac{E_1 (T_0 - T_w)}{R T_w^2},$$

and we obtain the dimensionless governing equation together with initial and boundary conditions as

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial y^2} + \lambda (1 + \varepsilon \theta)^m \left[e^{\left(\frac{\theta}{1 + \varepsilon \theta} \right)} + \beta e^{\left(\frac{r \theta}{1 + \varepsilon \theta} \right)} \right], \quad (2.5)$$

$$\theta(y, 0) = b, \quad (2.6)$$

$$\frac{\partial \theta}{\partial y}(0, t) = 0, \theta(1, t) = 0, \text{ for } t > 0 \quad (2.7)$$

where λ , ε , β , r , b represent the Frank-Kamenetskii parameter, activation energy parameter, two step exothermic reaction parameter, activation energy ratio parameter and the initial temperature parameter respectively. In the following section, Eqs. (2.5)-(2.7) are solved numerically using a semi-discretization finite difference method so as to convert resulting partial differential equations to ordinary differential equations.

^aCorresponding author: E-mail oladapo_anu@yahoo.ie, Tel. +23481385550

3.0 Computational Approach

The discretization of the governing equations is based on a linear Cartesian mesh and uniform grid on which finite-differences are taken. Firstly, a partition of the spatial interval $[0, 1]$ is introduced. We divide it into N equal parts and define grid size $\Delta y = 1/N$ and grid points $y_i = (i-1)\Delta y$, $1 \leq i \leq N+1$. The first and the second spatial derivatives in Eqs. (2.5)-(2.7) are approximated with second-order central differences. Let $\theta_i(t)$ be an approximation of $\theta(y_i, t)$, then the semi-discrete system for the problem reads:

$$\frac{d\theta_i}{dt} = \frac{1}{(\Delta y)^2} (\theta_{i+1} - 2\theta_i + \theta_{i-1}) + \lambda (1 + \varepsilon \theta_i)^m \left[e^{\left(\frac{\theta_i}{1+\varepsilon \theta_i}\right)} + \beta e^{\left(\frac{r\theta_i}{1+\varepsilon \theta_i}\right)} \right], \quad (3.1)$$

$$\text{with initial conditions } \theta_i(0) = b, \quad 1 \leq i \leq N+1. \quad (3.2)$$

The equations corresponding to the first and last grid points are modified to incorporate the boundary conditions, i.e.

$$\left. \frac{\partial \theta}{\partial y} \right|_{y=0} = \frac{\theta_2 - \theta_0}{2\Delta y} = 0, \quad \theta_{N+1} = 0. \quad (3.3)$$

In Eq. (3.1), there is only one independent variable, so they are ordinary differential equations. Since they are first order, and the initial conditions for all variables are known, the problem is an initial value problem. The MATLAB program ode45 is employed to integrate sets of differential equations using a fourth order Runge-Kutta method.

4. Discussion of results

We have assigned numerical values to the parameters encountered in the problem in order to get a clear insight into the thermal development in the system. At initial stage, the temperature of the slab is assumed to be the same as wall temperature and parameter $b=0$. It is very important to note that $\beta=0$ corresponds to a one step chemical reaction case; an increase in the value $\beta > 0$ signifies an increase in the two step chemical reaction activities in the system.

Fig. (2) illustrates the evolution of the temperature field in the system. For fixed values of various thermophysical parameters, the slab temperature increases rapidly with time until it attains its steady state value. Generally the temperature is maximum along the slab centerline and minimum at the wall satisfying the boundary conditions. Fig. (3) shows that the slab temperature is highest during bimolecular reaction and lowest for sensitized reaction. In Figs. (4) and (5), we observed that the slab temperature generally increases with increasing value of Frank-Kamenetskii parameter (λ) and two step reaction parameter. This can be attributed to an increase in the rate of internal heat generation activities due to chemical kinetics in the system.

5. Conclusion

We have examined the unsteady state of a two step exothermic reaction and our results show that the slab temperature is highest during bimolecular reaction and lowest for sensitized reaction. Similarly, the temperature increases across the slab as Frank- Kamenetskii parameter increases. In conclusion, we note that when $t=5$, the solution reached a steady state and that is why we fixed $t=5$ to investigate the effects of other parameters coming into the problem.

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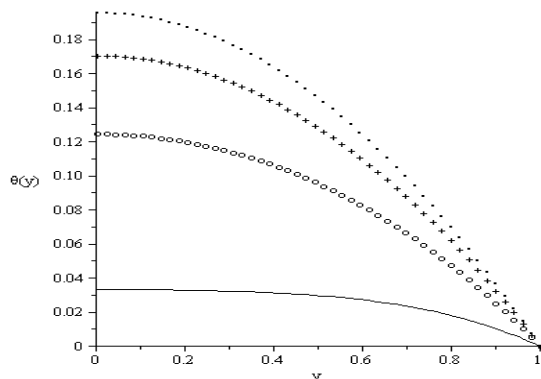


Fig.2: Temperature profiles: $b=0$; $\lambda=0.3$; $\varepsilon=0.4$; $\beta=0.1$; $m=0.5$; $r=0.1$; _____ $t=0.1$; oooooo $t=0.5$; +++++ $t=1$; $t=5$.

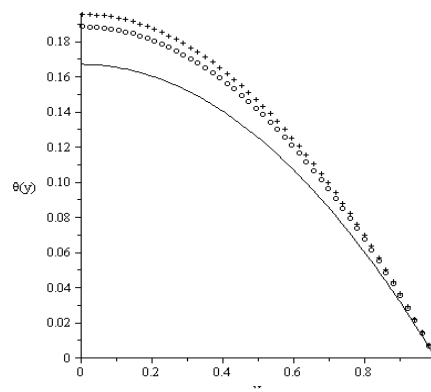


Fig.3: Temperature profiles: $b=0$; $\lambda=0.3$; $\varepsilon=0.4$; $\beta=0.1$; $t=5$; $r=0.1$; _____ $m=-2$; oooooo $m=0$; +++++ $m=0.5$

^aCorresponding author: E-mail oladapo_anu@yahoo.ie , Tel. +23481385550

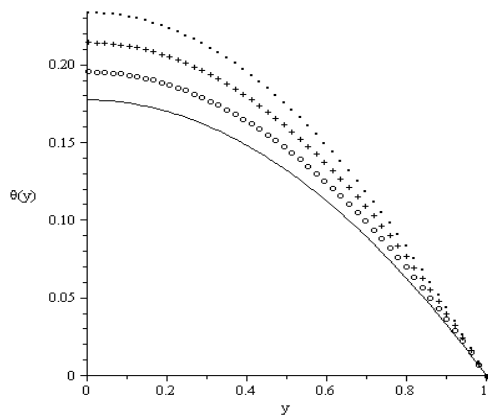


Fig.4: Temperature profiles: $b=0$; $\lambda=0.3$; $\varepsilon=0.4$;
 $t=5$; $m=0.5$; $r=0.1$; _____ $\beta=0$;
 ooooo $\beta=0.1$; +++++ $\beta=0.2$; $\beta=0.3$

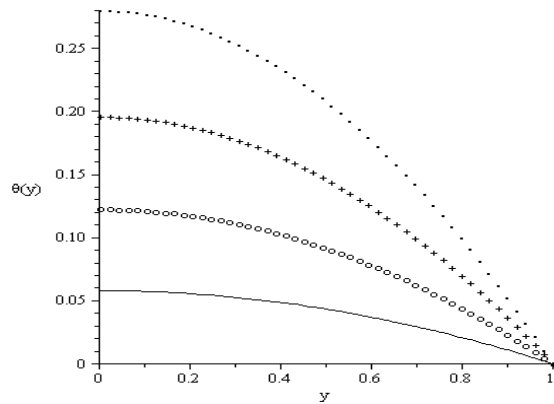


Fig.5: Temperature profiles: $b=0$; $\beta=0.1$;
 $\varepsilon=0.4$; $t=5$; $m=0.5$; $r=0.1$; _____ $\lambda=0.1$;
 ooooo $\lambda=0.2$; +++++ $\lambda=0.3$; $\lambda=0.4$

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^aCorresponding author: E-mail oladapo_anu@yahoo.ie , Tel. +23481385550