

Full Length Research Paper

Analysis of transient heating due to exothermic reaction in a stockpile of combustible material

B. H. Hamza¹, E. S. Massawe^{1*} and O. D. Makinde²

¹Department of Mathematics, University of Dar es Salaam, P. O. Box 35062, Tanzania.

²Institute for Advance Research in Mathematical Modelling and Computations, Cape Peninsula University of Technology, P. O. Box 1906, Bellville 7535, South Africa.

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In this paper, the transient heating in a stockpile of combustible material due to an exothermic reaction in the presence of convective heat loss to the ambient is analyzed. The transient heating in a slab due to an exothermic chemical reaction with the possibility of heat loss to the ambient is considered. The chemistry involved in the problem is simplified by assuming a one-step finite-rate irreversible Arrhenius kinetics. By introducing dimensionless variables into the equations, the governing nonlinear partial differential equations are solved numerically by method of lines (MOL), with finite difference schemes used for the discretisation of the spatial derivatives. Graphical results are presented and discussed quantitatively with respect to various embedded parameters controlling the systems. The results reveal that among others, the slab temperature increases gradually with time for a given set of parameters value until the steady state is achieved. The slab temperature is highest during bimolecular reaction in comparison to Arrhenius and sensitized types of chemical reaction. Moreover, an increase in the heat loss to the ambient enhances thermal stability of the system.

Key words: Transient heating, Arrhenius kinetics, variables.

INTRODUCTION

Theoretical study of transient heating in a slab of combustible material due to exothermic chemical reaction plays a significant role in many industrial applications (Lohrer et al., 2005). These include: Heavy oil recovery, storage of cellulosic materials, the pyrolysis of biomass and coal, the combustion of solids, waste incineration, coal gasification, etc. Without adequate knowledge of a reacting system, exothermic chemical process can accelerate, significantly leading to runaway reaction, possible explosion, economical losses and cause emission of carbon dioxide and of toxic gases, like carbon monoxide through incomplete combustion (Balakrishnan et al., 1969; Kamenetskii, 1969; Warnatz et al., 2001). Simmie (2003) presented a comprehensive review of chemical kinetic models for the heating-up of combustible materials. Meanwhile, analytical solutions of the highly nonlinear partial differential equations governing transient heating in a slab of combustible

Material due to exothermic reactions is usually impossible or extremely difficult to obtain. Hence in most

cases, a numerical solution approach is adopted (Makinde, 2004; Sadiq and Merkin, 1994; Bebernes and Eberly, 1989; Makinde and Moitsheki, 2010; Phiri and Makinde, 2010; Legodi and Makinde, 2011). In this paper, our objective is to perform a numerical study of transient heating in a slab of combustible material, in the presence of possible convective heat loss to the ambient.

ANALYSIS

The geometry of the problem is depicted in Figure 1. We consider the transient heating in a slab due to an exothermic chemical reaction with the possibility of heat loss to the ambient. The chemistry involved in the problem is simplified by assuming a one-step finite-rate irreversible Arrhenius kinetics.

Assuming no reactant consumption, the one dimensional heat balance nonlinear partial differential equation governing the system is given by (Balakrishnan et al., 1969; Makinde, 2004; Bebernes and Eberly, 1989).

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial y^2} + Q_1 A C_0 \left(\frac{KT}{vh} \right)^m e^{-\frac{E}{RT}} - \gamma(T - T_a) \quad (1)$$

*Corresponding author. E-mail: emassawe@uccmail.co.tz.

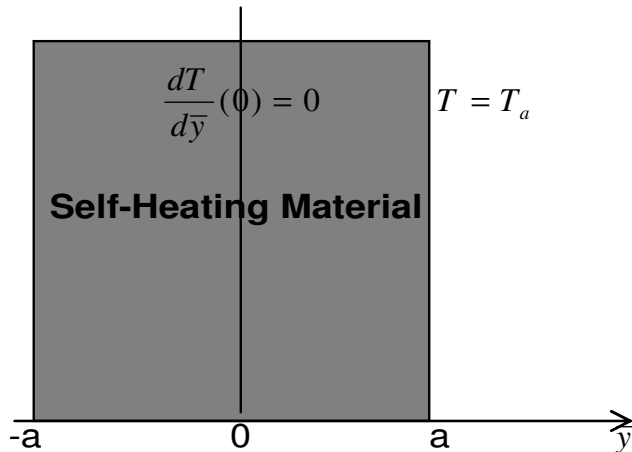


Figure 1. Geometry of the problem.

with the initial and boundary conditions as:

$$T(\bar{y}, 0) = T_0, \quad (2)$$

$$\frac{\partial T}{\partial \bar{y}}(0, \bar{t}) = 0, \quad T(a, \bar{t}) = T_a, \quad (3)$$

where T is the absolute temperature, T_a is the ambient temperature, \bar{t} is the time, ρ is the density, C_p is the specific heat at constant pressure, T_0 is the slab initial temperature, k is the thermal conductivity of the material, C_0 is the reactant concentration, Q_i is the exothermicity, A is the rate constant, E is the activation energy, R is the universal gas constant, h is the Planck's number, K is the Boltzmann's constant, ν is the vibration frequency, a is the slab half width, \bar{y} is the distance measured transverse direction, γ is the heat loss parameter and m is the numerical exponent such that $m = (-2, 0, 0.5)$ represent numerical exponent for sensitised, Arrhenius and bimolecular kinetics, respectively. We introduce the following dimensionless variables into Equations 1 to 3:

$$\theta = \frac{E(T - T_a)}{RT_a^2}, \quad \theta_0 = \frac{E(T_0 - T_a)}{RT_a^2}, \quad y = \frac{\bar{y}}{a}, \quad t = \frac{k\bar{t}}{\rho C_p a^2},$$

$$\varepsilon = \frac{RT_a}{E}, \quad \lambda = \frac{Q_i A E a C_0}{k R T_a^2} \left[\frac{K T_a}{\nu h} \right]^m e^{\frac{E}{R T_a}}, \quad \beta = \frac{a^2 \gamma}{k}, \quad (4)$$

and obtain the dimensionless governing equations as:

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial y^2} + \lambda(1 + \varepsilon \theta)^m e^{\frac{\theta}{1 + \varepsilon \theta}} - \beta \theta, \quad (5)$$

with

$$\theta(y, 0) = \theta_0, \quad (6)$$

$$\frac{\partial \theta}{\partial y}(0, t) = 0, \quad \theta(1, t) = 0, \quad (7)$$

where λ , ε , β and θ_0 represent the Frank-Kamenetskii parameter, activation energy parameter, heat loss parameter and initial slab temperature parameter. In the following section, Equations 5 to 7 are solved numerically using method of lines (Warnatz et al., 2001).

NUMERICAL PROCEDURE

The chemistry involved in the exothermic reactive process introduces stiffness and/or multiple time scales, so the availability of robust stiff ODE (ordinary differential equation) integrators gives an advantage to method of lines (Berzins and Ware, 1996). The governing Equation 5 with the initial and boundary conditions (Makinde, 2004; Sadiq and Merkin, 1994) is transformed into a system of ODEs using finite difference for the spatial derivative. The discretization is based on a linear cartesian mesh and uniform grid.

The spatial interval $0 \leq y \leq 1$ is partitioned into N equal parts with grid size $\Delta y = 1/N$ and grid points $y_i = (i-1)\Delta y$, $1 \leq i \leq N+1$. The first and second order spatial derivatives in Equations 5 to 7 are approximated with second-order central difference. Let $\theta_i(t)$ be the approximations of $\theta(y_i, t)$, then, the semi-discrete system for the problem becomes:

$$\frac{d\theta_i}{dt} = \frac{1}{(\Delta y)^2} (\theta_{i+1} - 2\theta_i + \theta_{i-1}) + \lambda(1 + \varepsilon \theta_i)^m \left[e^{\frac{\theta_i}{1 + \varepsilon \theta_i}} \right] - \beta \theta_i, \quad (8)$$

with initial conditions:

$$\theta_i(0) = \theta_0, \quad 1 \leq i \leq N+1. \quad (9)$$

The equations corresponding to the first and last grid points are modified to incorporate the boundary conditions; that is,

$$\left. \frac{d\theta}{dy} \right|_{y=0} = \frac{\theta_3 - \theta_1}{2\Delta y} = 0, \quad \theta_{N+1} = 0. \quad (10)$$

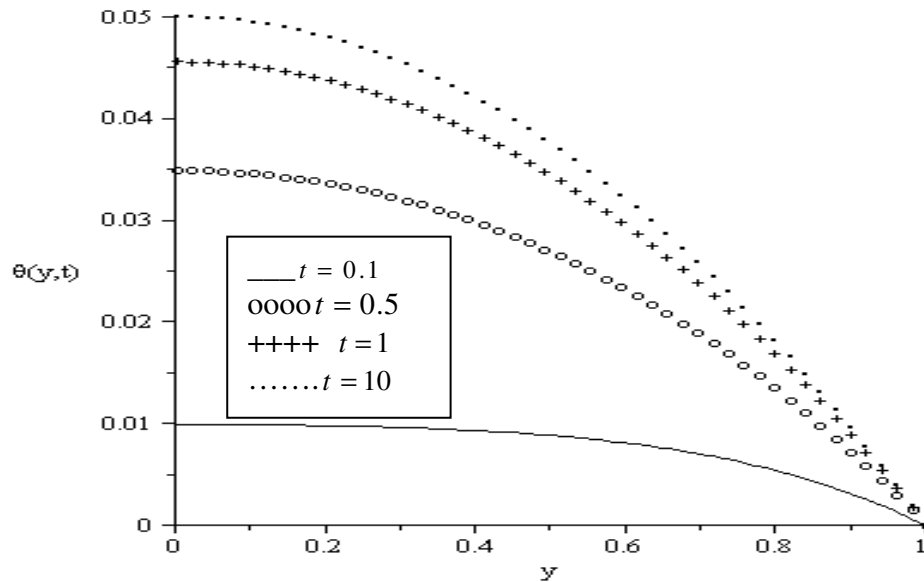


Figure 2. Temperature profiles showing the transient effect for $m = 0.5$, $\beta = \lambda = \varepsilon = 0.1$.

Equations 8 to 10 are first order initial value problem and contain only one independent variable. The inbuilt ODE45 program in Matlab can easily be employed to integrate the set of ordinary differential equations using a Runge-Kutta numerical method.

RESULTS AND DISCUSSION

In order to get a clear insight into the thermal development in the system due to an exothermic chemical reaction, we have assigned numerical values to the parameters encountered in the problem. At initial stage (that is, $t = 0$), the temperature of the slab is assumed to be equal to that of the ambient (that is, $\theta_0 = 0$) and there is no convective heat loss to the ambient. However at $t > 0$, the exothermic reaction in the system progresses, leading to heat generation and the possibility of heat loss from the system to the ambient since the temperature of the slab will be higher than that of the surrounding ambient. In Figures 2 to 6, we demonstrate the effects of various thermophysical parameters on the slab temperature profiles. Generally, the slab temperature is highest along its centerline and lowest at the surface due to convective heat loss to the ambient. Figures 2 and 3 illustrate the time evolution of the temperature field in the slab for a given set of fixed values for the embedded parameters. It is noteworthy that the slab temperature increases gradually with time until it attains its steady state value. Once its steady state temperature is attained, any further increase in the reaction time does not produce additional increase in the slab temperature. Figure 4 shows that the slab temperature is highest during bimolecular reaction

($m = 0.5$) and lowest for sensitized reaction ($m = -2$). This observation is in perfect agreement with the one reported by Makinde (2004) for the steady state exothermic reaction in a slab and the temperate profiles obtained also compares well with the one reported earlier in the literature. In Figure 5, we observe that the slab temperature decreases with an increase in the values of heat loss parameter (β). This clearly implies that an increase in the convective heat loss to the ambient will enhance thermal stability of the system and reduce the risk of thermal runaway problem. Figure 6 shows that the slab temperature increases with an increase in the parameter values of (λ). An increase in the value of Frank-Kamenetskii parameter (λ) indicates an increase in the slab internal heat generation due to exothermic chemical reaction in the system; this invariably leads to an elevation in the slab temperature. Moreover, it is important to note that a continuous increase in the reaction rate without considerable heat loss to the ambient may lead to an increase in heat accumulation within the system and the possibility of thermal runaway.

Conclusion

Analysis has been carried out to study the transient heating in a slab of combustible material due to exothermic chemical reaction in the presence of convective heat loss to the ambient. The nonlinear partial differential equation for the problem is solved numerically

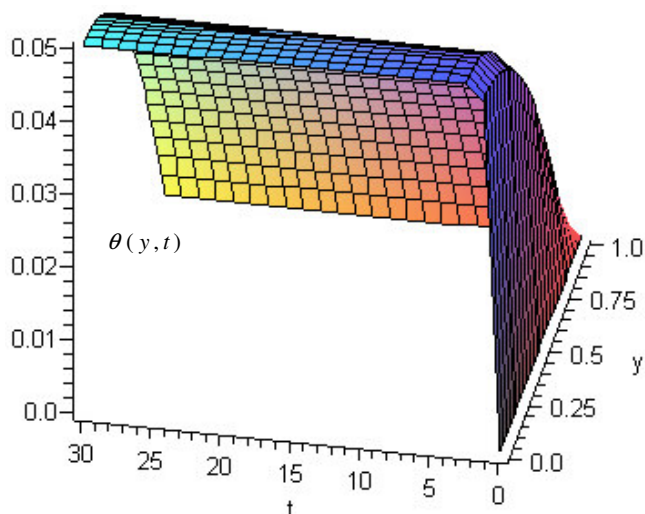


Figure 3. Three dimensional plot of temperature profiles for $m = 0.5$, $\beta = \lambda = \varepsilon = 0.1$.

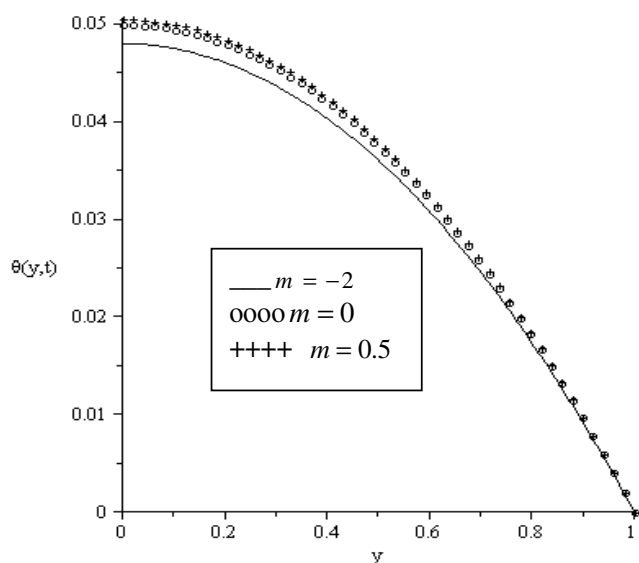


Figure 4. Temperature profiles showing the effect of reaction type index for $t = 10$, $\beta = \lambda = 0.1$, $\varepsilon = 0.5$.

using semi-discretization technique called method of lines. Our results reveal among others, the slab temperature increases gradually with time for a given set of parameters value until the steady state is achieved. The slab temperature is highest during bimolecular reaction in comparison with the Arrhenius and sensitized types of chemical reaction. Moreover, an increase in the heat loss to the ambient enhances thermal stability of the system. Finally, in the future we intend to extend the analysis in this present study to two and three dimensional problems in the presence of exothermic chemical reaction with radiative and convective heat loss.

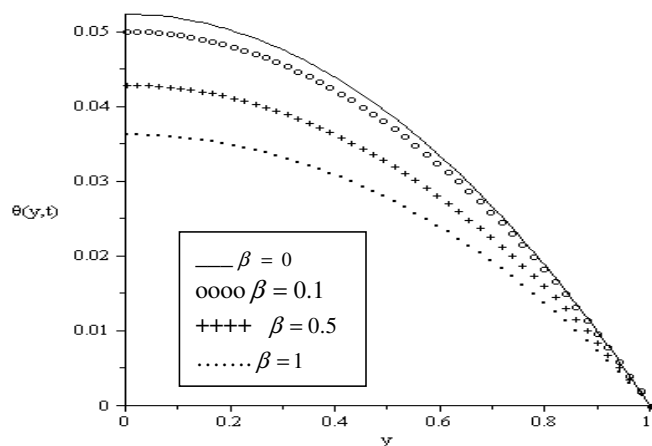


Figure 5. Temperature profiles showing the effect of heat loss for $t = 10$, $m = 0.5$, $\lambda = 0.1$, $\varepsilon = 0.1$.

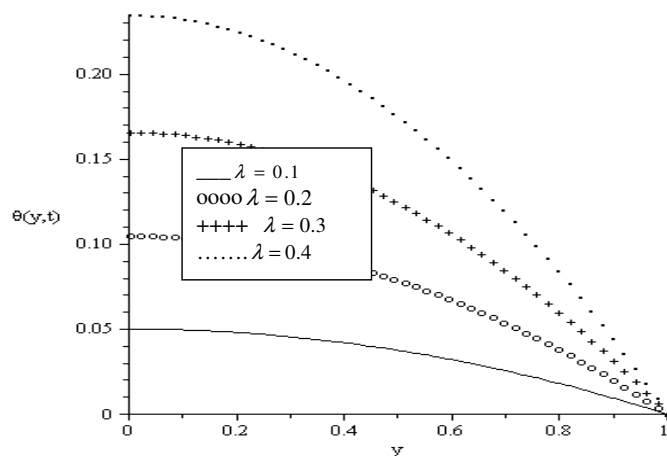


Figure 6. Temperature profiles showing the effect of increasing reaction rate for $t = 10$, $m = 0.5$, $\beta = 0.1$, $\varepsilon = 0.1$.

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