

Numerical Investigation of Thermal Stability in a Reactive Sphere of Variable Thermal Conductivity

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Abstract

Thermal stability in a stockpile of combustible material modelled in a spherical domain is investigated in this article. The reactive material of the sphere is considered with temperature dependent thermal conductivity and the sphere is assumed to lose heat to the ambient due to exothermic chemical reaction taking place within it. Also, a one-step finite rate irreversible Arrhenius kinetics is assumed to tackle the complicated chemical reaction taking place in this problem. We apply finite difference method (FDM) to solve numerically the differential equation governing the problem. FDM is very essential for spatial derivatives discretization. Heat transfer analysis for variation of kinetic parameters embedded within the system, against temperature, is presented graphically and the results are discussed accordingly.

Keywords: Transient heat, reactive sphere, FDM, exothermic chemical reaction

NOMENCLATURE

A	Rate constant [s^{-1}]
C	Reactant concentration [$kgmol^{-1}$]
E	Activation energy [$Jmol^{-1}$]
k	Thermal conductivity of the reacting sphere [$J s^{-1} m^{-1} K^{-1}$]
K	Boltzmann constant [$J K^{-1}$]
l	Planck number [$J s$]
m	Numerical exponent
Q	Heat of reaction [$J kg^{-1}$]
R	Universal gas constant [$J K^{-1} mol^{-1}$]
T	Absolute temperature of the sphere [K]
T_b	Surface temperature of the sphere [K]
\bar{r}	Sphere radial distance [m]

Greek Symbols

ε	Dimensionless activation energy parameter
θ	Dimensionless temperature
λ	Modified Frank-Kamenetskii parameter
ν	Vibration frequency [s^{-1}]

1. INTRODUCTION

A stockpile of reactive material modelled in a spherical geometry is considered in this investigation. The stockpile is considered with variable thermal conductivity, that is, thermal conductivity that varies exponentially with temperature. The reactive material of the stockpile are carbon containing substances, such as cotton, hay, wool, paper, or industrial wastes. The reactive material reacts spontaneously with oxygen trapped inside the stockpile to produce, mainly, heat and carbon dioxide, when complete combustion is assumed. Heat and carbon dioxide released are of environmental importance since about 80% of carbon dioxide emitted in this type of reaction contributes to Greenhouse effect [1, 2]. Should the heat release in this exothermic chemical reaction exceed its release to the surrounding environment, the temperature of the system may raise rapidly and result into thermal runaway with spontaneous-ignition taking place [3,4,5].

Spontaneous-ignition results into fires that are hazardous to living species, environment and industry [6, 7]. Part of the application of thermal stability investigation is in the improvement of the design and operation of some industrial and engineering appliances. It has been observed that the quality of some industrial products is affected by internal heat generation due to exothermic chemical reaction after coating or lamination [8, 9]. The exothermic chemical reaction that results with spontaneous-combustion in this investigation, is very complicated and involves many radicals [10, 11]. To simplify this complicated chemistry, a one-step decomposition kinetics is used to model this phenomenon mathematically using partial differential equation for heat transfer [12]. It is not possible to obtain an exact solution to the differential equation governing the problem because of the nonlinear interactions of reacting species [13,

14]. Therefore the governing equation is solved numerically by using semi-implicit FDM and Maple software is used to give solutions graphically.

The objective of this article is to investigate thermal stability in a spherical domain of combustible material with variable thermal conductivity, by looking at the behavior of different kinetic parameters embedded within the system in response to increase in temperature. The article arrangement is as follows: section 2 includes mathematical formulation, section 3 presents the numerical method applied, and detailed discussion of results and graphical solutions to the problem due to various thermo-physical parameters embedded within the system are outlined in section 4.

2. MATHEMATICAL FORMULATION

A stockpile of combustible material modelled in a spherical domain with temperature dependent thermal conductivity k is considered. The stockpile is assumed to be subjected to a one-step Arrhenius kinetics with the possibility of heat loss to the ambient. Fig. 1 depicts the geometry of the problem.

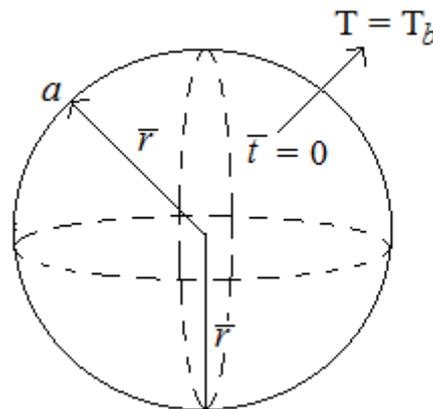


Figure 1: Geometry of the problem.

Neglecting the reactant consumption, the one-dimensional governing equation where the sphere of radius $\bar{r} = a$, with initial temperature, $T = T_0$ and the surface temperature made equal to T_b for time $\bar{t} > 0$ is given by [6]:

$$\rho c_p \frac{\partial T}{\partial \bar{t}} = \frac{1}{\bar{r}^2} \frac{\partial}{\partial \bar{r}} \left(k(T) \bar{r}^2 \frac{\partial T}{\partial \bar{r}} \right) + QAC \left(\frac{KT}{vl} \right)^m e^{-E/RT} - \phi(T - T_b). \tag{1}$$

The initial condition is

$$T(\bar{r}, 0) = T_0, \tag{2}$$

with boundary conditions

$$\frac{\partial T}{\partial \bar{r}}(0, \bar{t}) = 0; \quad T(a, \bar{t}) = T_b. \quad (3)$$

Here, T is the sphere's absolute temperature, T_0 the initial temperature of the sphere, T_b is the ambient temperature, ρ is the density, c_p is the specific heat at constant pressure, Q is the heat of reaction, A is the rate constant, C is the reactant concentration, K is the Boltzmann's constant, ν is the vibration frequency, φ is the heat loss parameter, l is the Planck's number, E is the activation energy, R is the universal gas number, m is the numerical exponent such that $m = -2, 0, 0.5$ represents sensitized, Arrhenius and bimolecular kinetics, respectively [1,2,3,6,7]. The thermal conductivity of the material is assumed to increase with temperature exponentially and is given as

$$k(T) = \tau e^{b(T-T_b)}, \quad (4)$$

where τ is the material thermal conductivity at the ambient temperature T_b and b is the thermal conductivity variation parameter [6]. The following dimensionless parameters are introduced to equations (1) – (4):

$$\theta = \frac{E(T-T_b)}{RT_b^2}, \quad \theta_0 = \frac{E(T_0-T_b)}{RT_b^2}, \quad r = \frac{\bar{r}}{a}, \quad \beta = \frac{bRT_b^2}{E}, \quad t = \frac{\bar{t}}{\rho c_p a^2},$$

$$\varepsilon = \frac{RT_b}{E}, \quad \alpha = \frac{a^2 \varphi}{\tau}, \quad \lambda = \left(\frac{KT_b}{\nu l}\right)^m \frac{QAEa^2C}{\tau RT_b^2} \exp\left(-\frac{E}{RT_b}\right). \quad (5)$$

Equations (1) – (4) take the following forms:

$$e^{-\beta\theta} \frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial r^2} + \frac{2}{r} \frac{\partial \theta}{\partial r} + \beta \left(\frac{\partial \theta}{\partial r}\right)^2 + \lambda(1 + \varepsilon\theta)^m e^{\frac{\theta(1-\beta-\varepsilon\beta\theta)}{1+\varepsilon\theta}} - \alpha\theta e^{-\beta\theta} \quad (6)$$

with the initial and boundary conditions given as

$$\theta(r, 0) = \theta_0, \quad \frac{\partial \theta}{\partial r}(0, t) = 0, \quad \theta(1, t) = 0, \quad (7)$$

where θ is the dimensionless temperature, θ_0 is the dimensionless initial temperature, λ is the Frank-Kamenetskii parameter, also called the rate of reaction parameter, ε is the activation energy parameter, r is the dimensionless radial distance, α is the dimensionless heat loss parameter and β is the variable thermal conductivity parameter.

3. NUMERICAL APPROACH

Equations (6) subject to conditions (7) may be considered as an initial boundary value problem and are solved numerically using a semi-discretization finite difference method known as method of lines [15, 16]. A partition of the spatial interval $0 \leq r_i \leq 1$ into N equal parts is introduced such that the grid size $\Delta r = 1/N$ and grid points $r_i = (i-1)\Delta r$, $1 \leq i \leq N+1$. Both first and second spatial derivatives in equation (6) are

approximated with second-order central finite differences. Let $\theta_i(t)$ be the approximation of $\theta(r_i, t)$, then the semi-discrete system for the problem becomes

$$e^{-\beta\theta_i} \frac{d\theta_i}{dt} = \frac{1}{\Delta r^2}(\theta_{i+1} - 2\theta_i + \theta_{i-1}) + \frac{1}{r_i \Delta r}(\theta_{i+1} - \theta_{i-1}) + \frac{\beta}{4\Delta r^2}(\theta_{i+1} - \theta_{i-1})^2 + \lambda(1 + \varepsilon\theta_i)^m e^{\frac{\theta_i(1-\beta-\varepsilon\beta\theta_i)}{(1+\varepsilon\theta_i)}} - \alpha\theta_i e^{-\beta\theta_i} = 0, \tag{8}$$

with initial conditions given as

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

The equations corresponding to the first and last grid points are modified to incorporate the boundary conditions as follows

$$\theta_1 = \theta_0, \quad \theta_{N+1} = 0. \tag{10}$$

There is only one independent variable in the equation (8), so they are first order nonlinear ordinary differential equations (ODE) with known terminal conditions. We then solve the initial value problem iteratively using a fourth order Runge-Kutta-Fehlberg integration technique [16] implemented on Computer using MAPLE software. The results are displayed graphically and in tabular form in the following section.

4. RESULTS AND DISCUSSION

In this section effects of various kinetic parameters on temperature behavior are presented. Unless otherwise stated, the following parameters are used:

$$m = 0.5, n = 1, \beta = 1, \lambda = 1, \alpha = 1, \varepsilon = 0.1, t = 10.$$

4.1 Effects of kinetic parameters on temperature

It is assumed that at the initial stage, $t = 0$, the temperature of the sphere is equal to that of the surrounding. But at $t > 0$, the temperature of the sphere exceeds that of the ambient due to self-heating that is caused by the trapped oxygen reacting with the reactive material within the sphere. Figures 2 – 5 illustrate the behavior of the temperature in response to variation of thermo-physical parameters embedded in the system. The Figures 2a - b illustrate the behavior of temperature as time t increases while other thermo-physical parameters, $\lambda, \varepsilon, \beta, m$ and α , are kept constant. The general trend is that the temperature of the sphere is highest along the center and lowest at its surface as heat loss to the ambient takes place for $t > 0$. We observe also from Figs. 2a - b that the sphere’s temperature attains its steady state value, and once the steady state value is reached, no further increase in temperature is experienced.

In Figure 3, we observe how temperature varies as λ , the rate of reaction parameter, increases. An increase in λ shows a corresponding increase in temperature fields of the sphere due to exothermic chemical reaction taking place within the system. As a result,

we see high values of temperature attained, and if λ keeps on increasing without appropriate loss of heat to the surrounding, more heat can accumulate within the system to cause self-ignited fires. We also see the same result of temperature increase in Figure 4 as the activation energy parameter ε increases. In this case, ε , has no strong effect on temperature behavior as compared to λ . If ε is increased with small values, its effect on temperature behavior may not be observed, hence the high values employed to show the effect. This applies also for β in Figure 6.

A different scenario is observed in Figure 5, where an increase in α shows a decrease in temperature fields. This parameter indicates that considerable heat loss to the ambient encourages the system's thermal stability and that the risk of self-ignited fires is minimized.

Figure 7 indicates the variation of m , for values -2, 0 and 0.5, where $\varepsilon = 0.5$. We observe also that the increase in m gives the corresponding increase in temperature profiles. The next section shows that variation of m from -2 to 0.5 has also an effect on thermal stability of the system.

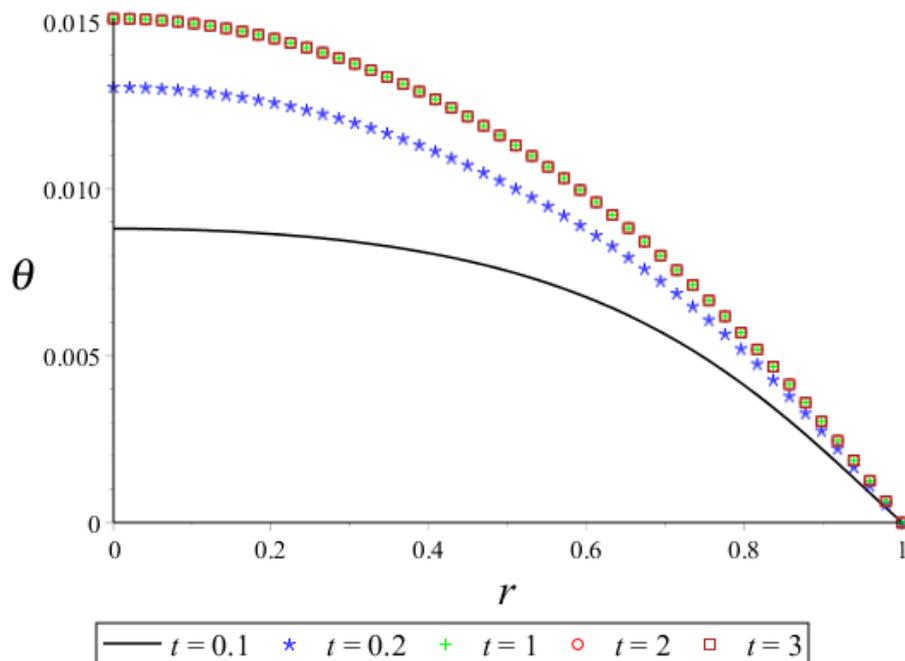


Figure 2a: Temperature profiles with time

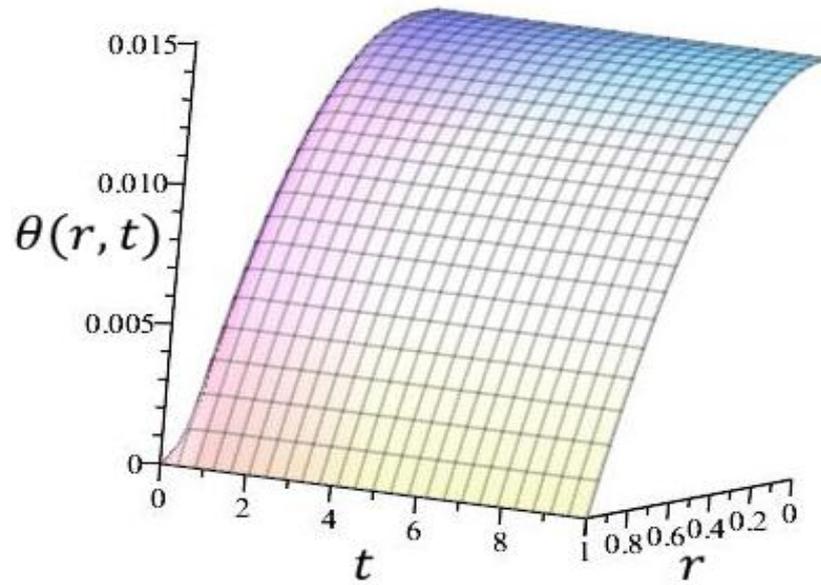


Figure 2b: 3-D Temperature profiles with time

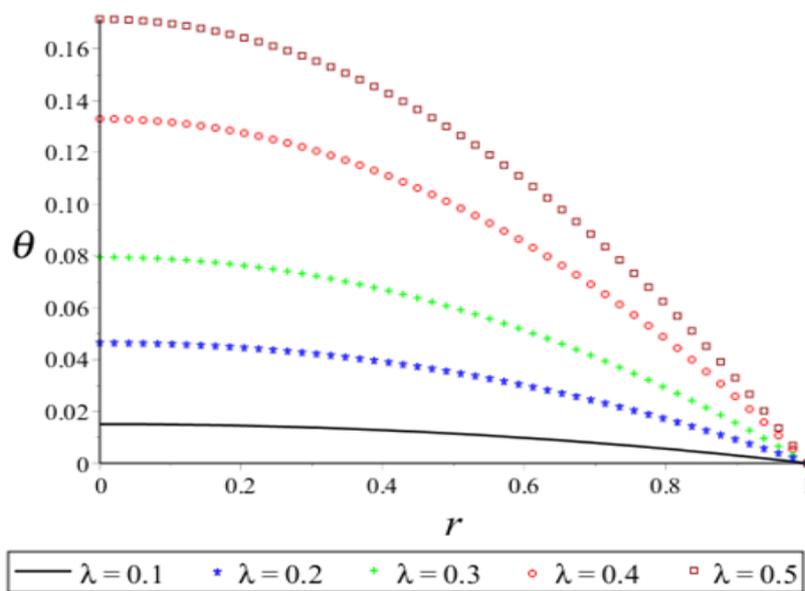


Figure 3: Temperature variation with λ .

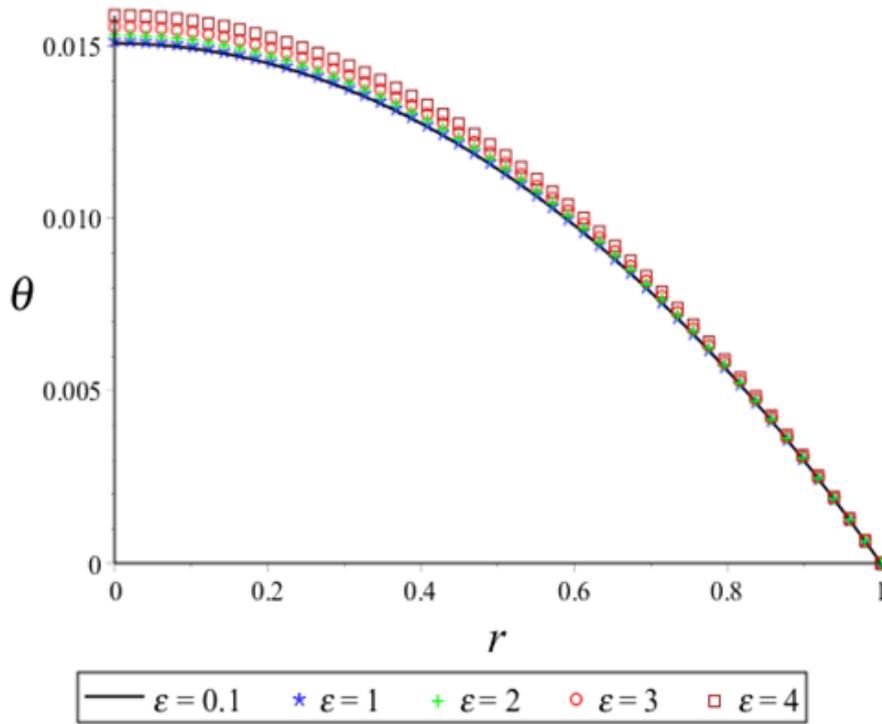


Figure 4: Temperature variation with ϵ .

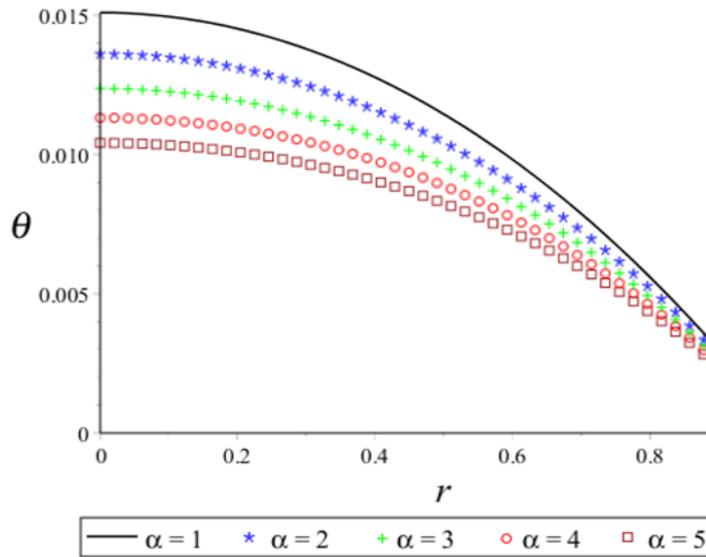


Figure 5: Temperature variation with α .

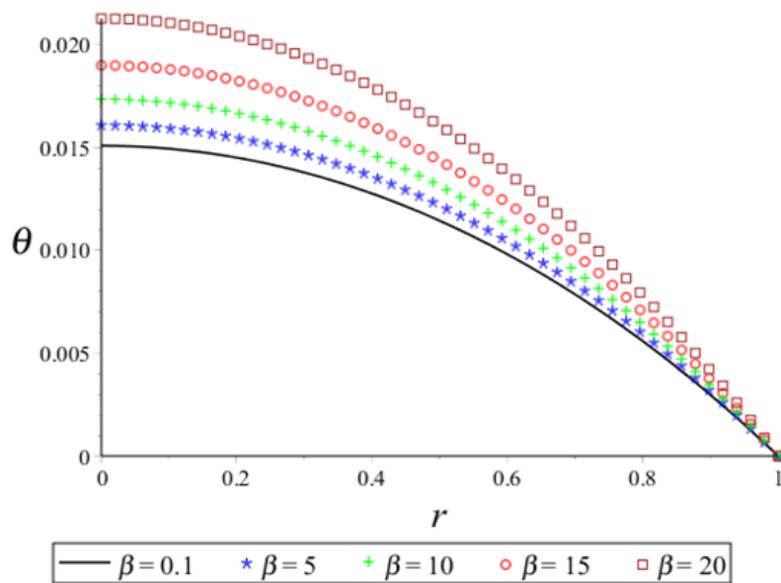


Figure 6: Temperature variation with β .

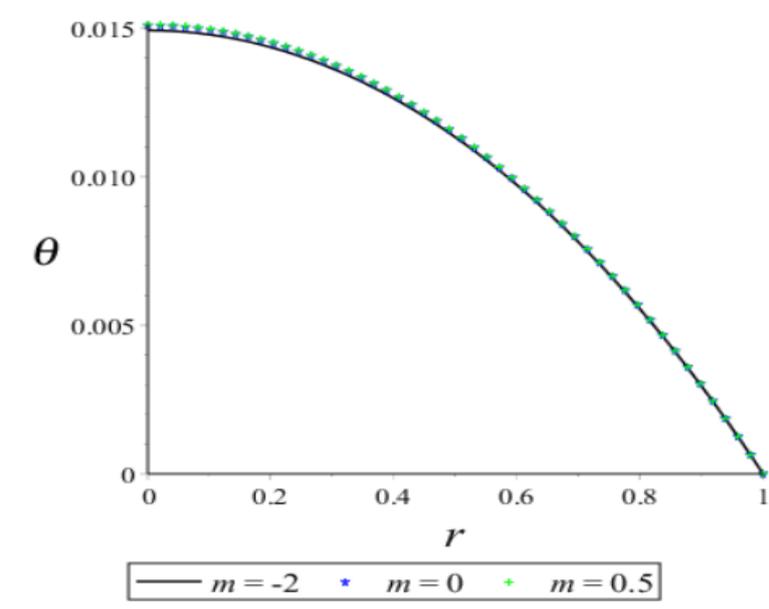


Figure 7: Temperature variation with m .

4.2 Thermal stability analysis

Here, we analyze thermal stability by plotting the Nusselt number (Nu) against the reaction rate parameter (λ). The results are illustrated in Figures 8 – 11 and Table 1 for the following parameters $\varepsilon, \alpha, \beta$ and m . Thermal stability is illustrated by the longest

graph that corresponds to the highest value of λ . We observe from Figures 8 – 9 that an increase in the parameter values of ε and α give a corresponding increase on λ values. This means that thermal stability is attained by keeping highest values of these parameters. A different scenario is observed in Figures 10 – 11 where an increase in m and β results in the decrease of λ . This means that thermal stability is attained at lowest values of both m and β .

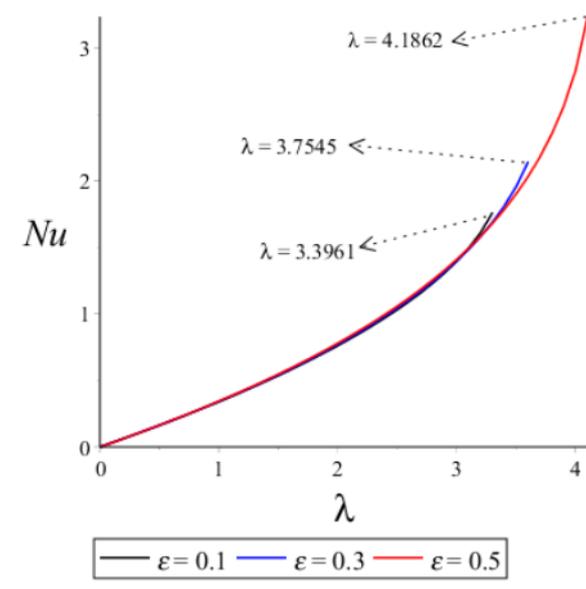


Figure 8: ε on thermal stability

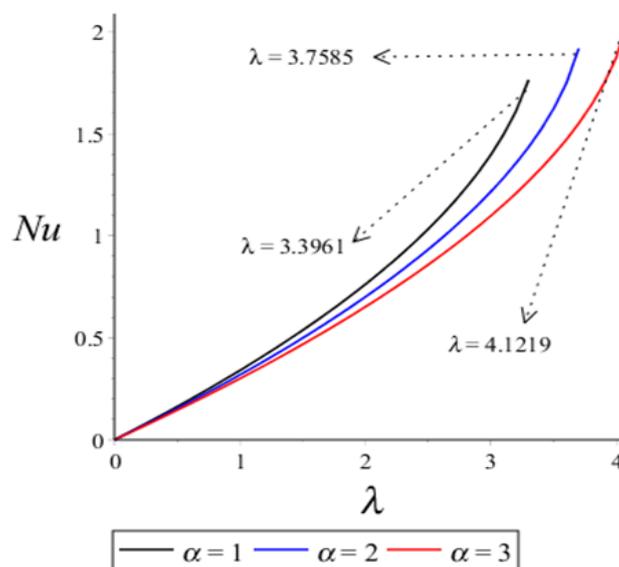


Figure 9: α on thermal stability.

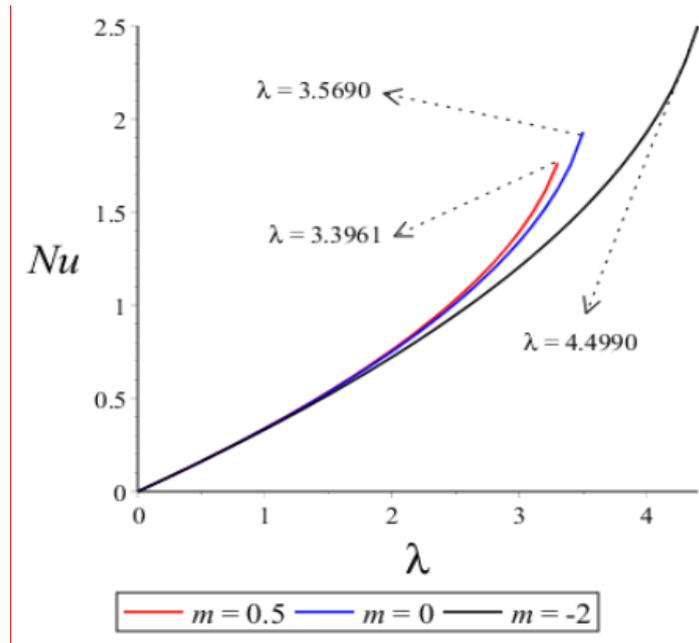


Figure 10: m on thermal stability

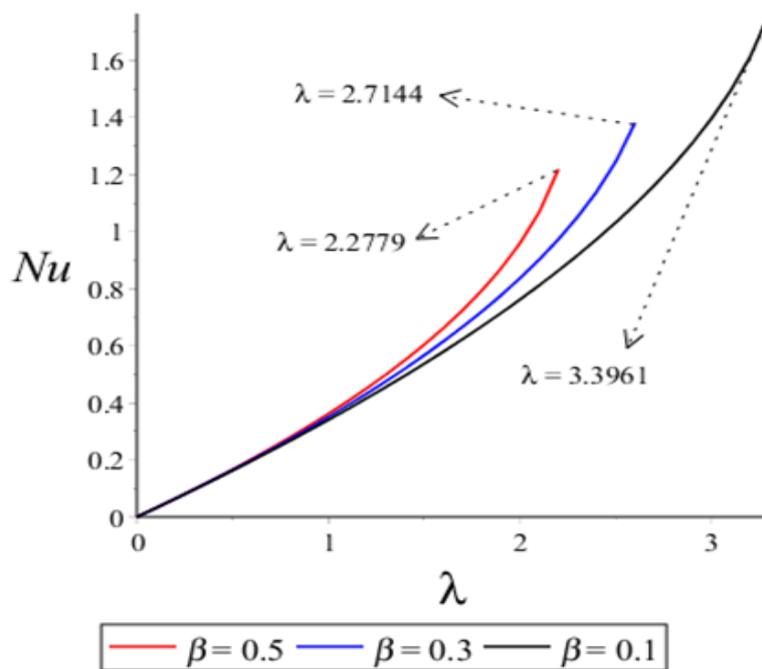


Figure 11: β on thermal stability.

Values obtained for Nu and λ for varied α , ε , m and β respectively, are given in Table 1 below.

Table 1: Numerical values showing effects of kinetic parameters on thermal criticality values.

α	ε	m	β	Nu	λ
1	0.1	0.5	0.1	2.10826	3.3961
2	0.1	0.5	0.1	2.16914	3.7585
3	0.1	0.5	0.1	2.22860	4.1219
1	0.3	0.5	0.1	2.87478	3.7585
1	0.5	0.5	0.1	4.21919	4.1862
1	0.1	0	0.1	2.23275	3.5690
1	0.1	-2	0.1	2.95814	4.4990
1	0.1	0.5	0.3	1.74459	2.7144
1	0.1	0.5	0.5	1.51607	2.2779

5. CONCLUSION

Analysis of transient heat in a stockpile of reactive material was investigated in this case. The study was modelled in a spherical domain. The thermo-physical parameters embedded within the system that have an effect on temperature behavior during exothermic chemical reaction in a sphere, were identified as λ , ε , β , m and α for $t > 0$. It was found that an increase on parameters λ , ε , β and m increases the temperature of the sphere during the exothermic chemical reaction. The parameter α shows an opposite effect, which is of importance to attain thermal stability of the system. The significance of this theoretical investigation of self-igniting processes is to provide a cheaper and simpler way of understanding factors that enhance temperature increases or vice-versa, by using mathematical approach. This study can be extended to two-step reactive sphere of variable thermal conductivity.

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