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Oxygen Depletion and Thermal Stability Analysis in a Reactive Sphere of Variable Thermal Conductivity

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Abstract

The depletion of oxygen in a stockpile of combustible material is investigated in this study. The process is modeled in a spherical domain of thermal conductivity that is temperature dependent, where oxygen trapped within the system reacts spontaneously with carbon containing material of the stockpile. The spontaneous reaction is due to exothermic chemical reaction taking place within the stockpile when oxygen is used up and carbon dioxide, heat and water are part of products. The process is assumed also to undergo complete combustion. The complicated combustion process is tackled by assuming a one-step irreversible chemical reaction. The derived partial differential equations for heat transfer and oxygen consumption mass transfer are numerically solved using Finite Difference Method (FDM). Effects of embedded kinetic parameters on temperature and reactant consumption behaviors are depicted graphically and discussed accordingly.

Keywords: Oxygen depletion, heat transfer, reactive sphere, FDM, variable thermal conductivity.

INTRODUCTION

The depletion of oxygen has drawn the attention of many researchers because oxygen is very important to all living species. Lu etal. [1], investigated oxygen depletion in upper waters of oceans, which is commonly associated with poor ventilation and respired carbon storage linked to carbon dioxide of the atmosphere. Kurre and Maier [2] also discussed how oxygen depletion triggers switching between discreet speed modes of polymeric bacterial appendages that affect interaction of host cell, motility, biofilm formation, and transfer of horizontal gene. Oxygen depletion in spontaneous ignition is of environmental interest because during its consumption carbon dioxide and heat are released to the atmosphere to contribute to the Greenhouse effect. Emissions of carbon dioxide and heat are the major causes of climate and global warming [3, 4]. The previous studies showed that almost 80% of Greenhouse effect is caused by carbon dioxide emitted from stockpiles of reactive materials [5, 6, 7]. Reactive stockpiles may consist of coal, cotton, hay, wood, or any carbon containing material. Spontaneous ignition in a reactive stockpile takes place due to exothermic chemical reaction when the stockpile carbon containing material reacts automatically with oxygen trapped within the stockpile.

Thermal stability investigation of a combustible material in a stockpile is also of importance. It should be noted that self–ignition takes place when the rate of heat generated due to exothermic chemical reaction exceeds that of heat loss to the environment [8, 9, 10]. This process may lead to phenomenon called thermal explosion which was intensively explored by Frank-Kamenetskii [11]. Analysis of thermal explosion in a combustible material is helpful to determine critical values which are not to be exceeded to avoid explosion from taking place in self-ignited processes. To do this analysis, the Nusselt number, which is the dimensionless heat transfer rate at the sphere's surface, is plotted against the Frank-Kamenetskii parameter, also called the rate of reaction parameter, for some embedded thermo-physical parameters of the system. Investigation of oxygen depletion and thermal stability was done in [6, 12, 13] for both a long cylindrical pipe and a reactive slab. In this investigation we consider modelling our problem in a reactive sphere. The article setup is done as follow, in section 2 detailed mathematical modelling is outlined, section 3 gives the numerical method approach used to solve the nonlinear differential equations governing the problem. Section 4 outlines results and discussion of effects of different embedded thermo-physical parameters on temperature and oxygen depletion. The conclusion is discussed in section 5.

2. MATHEMATICAL MODELLING

A complete combustion process in a reactive stockpile where the system undergoes an n^{th} oxidation chemical reaction and subjected to convective heat loss is assumed in this study. The investigation is modelled in a spherical domain of variable thermal conductivity. A one-step finite rate irreversible chemical kinetics mechanism between the material and the oxygen of the air is assumed and it is expressed by the following formula:

$$\mathrm{C}_i\mathrm{H}_j + \left(i + \frac{j}{4}\right)\mathrm{O}_2 \rightarrow i\mathrm{CO}_2 + \left(\frac{j}{2}\right)\mathrm{H}_2\mathrm{O} + \text{heat}. \tag{1}$$

Convective heat loss at the surface of the sphere obeys Newton's law of cooling and it is generally expressed by $-\frac{h}{k}[T - T_b]$, where h is the heat transfer coefficient and k is the thermal conductivity of the material that varies with temperature according to the formula:

$$k = \tau e^{b(T-T_b)}, \tag{2}$$

where τ is the material thermal conductivity at the ambient temperature T_b, b is the thermal conductivity variation parameter [6] and T is the sphere temperature. Figure 1 below illustrates the geometry of the problem.

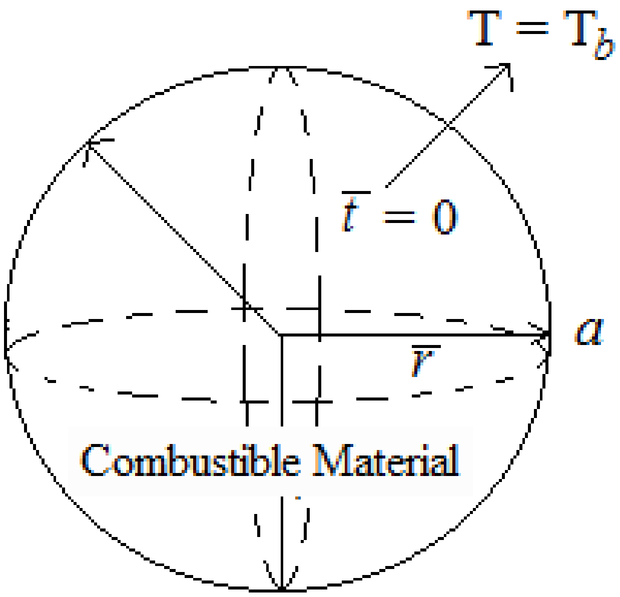

Figure 1: Geometry of the problem.

The nonlinear partial differential equations describing temperature, oxygen concentration and carbon dioxide emission in the combustible material can be written as [13,14]

$$\rho c_p \frac{\partial T}{\partial \bar{t}} = k \frac{1}{\bar{r}^2} \frac{\partial}{\partial \bar{r}}\left(\bar{r}^2 \frac{\partial T}{\partial \bar{r}}\right) + QA\left(\frac{KT}{vl}\right)^m (C - C_0)^n exp\left(\frac{-E}{RT}\right), \tag{3}$$

$$\frac{\partial C}{\partial \bar{t}} = D \frac{1}{\bar{r}^2} \frac{\partial}{\partial \bar{r}}\left(\bar{r}^2 \frac{\partial C}{\partial \bar{r}}\right) - A\left(\frac{KT}{vl}\right)^m (C - C_0)^n exp\left(\frac{-E}{RT}\right), \tag{4}$$

with initial conditions

$$T(\bar{r}, 0) = T_0, \quad C(\bar{r}, 0) = 0.5C_b. \tag{5}$$

Boundary conditions at the center of the sphere are

$$\frac{\partial T}{\partial \bar{r}}(0, \bar{t}) = \frac{\partial C}{\partial \bar{y}}(0, \bar{t}) = 0, \tag{6}$$

and the surface are

$$\frac{\partial T}{\partial \bar{r}}(a,\bar{t}) = -\frac{h_1}{k}[T(a,\bar{t}) - T_b],$$

$$\frac{\partial C}{\partial \bar{r}}(a,\bar{t}) = -\frac{h_2}{D}[C(a,\bar{t}) - C_b]. \quad (7)$$

Here C is the oxygen concentration, C_b is the oxygen concentration in the surrounding air, $\bar{t}$ is the time, T_0 is the slab initial temperature, C_0 is the initial concentration of oxygen in the slab, ρ is the density, c_p is the specific heat at constant pressure, D is the diffusivity of oxygen in the sphere, Q is the heat of reaction, A is the rate constant, E is the activation energy, R is the universal gas constant, l is the Planck number, v is the vibration frequency, K is the Boltzmann constant, $a = \bar{r}$ is the radial distance, h_1 is the heat transfer coefficient between the sphere and its surroundings, h_2 is the oxygen transfer coefficient between the sphere and its surroundings, n is the order of exothermic chemical reaction, and $m \in \{-2,0,0.5\}$ is the numerical exponent such that $m = -2$ represents the Sensitized kinetics, Arrhenius kinetics is represented by $m = 0$ and $m = 0.5$ is for Bimolecular kinetics, as indicated in [1,2,6,13,14]. The following dimensionless parameters are introduced into the set of Eqs. (3) – (7):

$$\left.\begin{aligned} &\theta = \frac{E(T-T_0)}{RT_0^2},\ \ \theta_b = \frac{E(T_b-T_0)}{RT_0^2},\ \ \Phi = \frac{C-C_0}{C_b-C_0}, \\ &Bi_1 = \frac{ah_1}{k},\ Bi_2 = \frac{ah_2}{D}, \beta = \frac{bRT_b^2}{E} \\ &\beta_1 = \frac{\rho c_p RT_0^2}{QEC_b}, \qquad \lambda = \left(\frac{KT}{vl}\right)^m \frac{QAEa^2C_b^n}{kRT_0^2} exp\left(\frac{-E}{RT}\right), \\ &r = \frac{\bar{r}}{a},\ \ t = \frac{k\bar{t}}{c_p\rho a^2},\ \ \varepsilon = \frac{RT_0^2}{E},\ \ \alpha = \frac{D\rho c_p}{k}, \end{aligned}\right\} \quad (8)$$

to obtain the following dimensionless governing equations:

$$e^{-\beta\theta}\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial r^2} + \frac{2}{r}\frac{\partial\theta}{\partial r} + \beta\left(\frac{\partial\theta}{\partial r}\right)^2 + \lambda(1+\varepsilon\theta)^m e^{\left(\frac{\theta}{1+\varepsilon\theta}\right)} e^{-\beta\theta} \quad (9)$$

$$\frac{\partial\Phi}{\partial t} = \alpha\left(\frac{\partial^2\Phi}{\partial r^2} + \frac{2}{r}\frac{\partial\Phi}{\partial r}\right) - \lambda\beta_1(1+\varepsilon\theta)^m e^{\left(\frac{\theta}{1+\varepsilon\theta}\right)} e^{-\beta\theta} \quad (10)$$

The corresponding initial conditions then become

$$\theta(r,0) = 0,\ \ \Phi(r,0) = 0.5, \quad (11)$$

and the boundary conditions are

$$\frac{\partial\theta}{\partial r}(0,t) = \frac{\partial\Phi}{\partial r}(0,t) = 0,$$

$$\frac{\partial\theta}{\partial r}(1,t) = -Bi_1[\theta(1,t) - \theta_b]e^{-\beta\theta},$$

$$\frac{\partial \Phi}{\partial r}(1,t) = -Bi_2[\Phi(1,t) - 1], \tag{12}$$

where λ is the Frank-Kamenetskii parameter, ε is the activation energy parameter, β_1 is the oxygen consumption rate parameter, α is the oxygen diffusivity parameter, Bi_1 and Bi_2 represent the thermal Biot number and oxygen Biot number respectively.

3. NUMERICAL APPROACH

The equations (9) – (12) are solved numerically by FDM algorithm that applies a mesh of nodes. Appropriate approximation of the governing equation is done by also introducing the time coordinate, to create another mesh of points in time. The explicit scheme is used with the space domain subdivided into equal size of subintervals to give a mesh of points. The forward difference approximation is applied for the time derivative and the centered difference formula is used for the spatial derivatives.
The difference formula for equations (9) – (10) is thus:

$$e^{-\beta\theta}\frac{d\theta_i}{dt} = \frac{1}{\Delta r^2}(\theta_{i+1} - 2\theta_i + \theta_{i-1}) + \frac{1}{2r_i\Delta r}(\theta_{i+1} - \theta_{i-1}) + \beta\left(\frac{\theta_{i+1} - \theta_{i-1}}{\Delta r}\right)^2 + \lambda(1 + \varepsilon\theta_i)^m e^{\left(\frac{\theta_i}{1+\varepsilon\theta_i}\right)} e^{-\beta\theta_i} \tag{13}$$

$$\frac{d\Phi_i}{dt} = \frac{1}{\Delta r^2}(\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}) + \frac{1}{2r_i\Delta r}(\Phi_{i+1} - \Phi_{i-1}) + \lambda(1 + \varepsilon\theta_i)^m e^{\left(\frac{\theta_i}{1+\varepsilon\theta_i}\right)} e^{-\beta\theta_i} \tag{14}$$

Initial condition is given as

$$\theta_i(0) = \theta_0. \tag{15}$$

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

$$\theta_1 = Bi_1\theta_i, \theta_{N+1} = -Bi_2\theta_i e^{-\beta\theta_i} \tag{16}$$

MAPLE software was used to solve equation. The results are displayed graphically and in tabular form in the following section.

4. RESULTS AND DISCUSSION

In this section effects of variation of thermo-physical parameters on temperature and oxygen depletion are depicted and graphically and discussed accordingly. Unless or otherwise stated, the following parameter values were used: $\lambda = 1, m = 0.5, n = 1, \beta = 0.1, \beta_1 = 0.1, \alpha = 1, \varepsilon = 0.1, Bi_1 = 1, Bi_2 = 1$.

4.1 Effects of thermo-physical parameters on temperature

In this subsection we discuss parameters variation on temperature as depicted in Figures 2 – 9. The figures help us to understand the effect of each parameter on the temperature of the system during combustion process. Figures 2 – 5 show that an increase in the parameters λ, ε, m and α show a corresponding increase in temperature profiles. These parameters enhance the exothermic chemical reaction which is the main cause of self-ignition process. The parameters also indicate an increase in the sphere's internal heat generation due to exothermic chemical reaction which makes the temperature of the system to be elevated. In general, the temperature is highest at the center of the sphere and lowest at the surface. A different scenario is observed in Figures 6 – 9, where an increase in parameters β, n, Bi_1 and β_1 show a decrease in the temperature profiles. These parameters enable us to understand that as their values are kept very high, exothermic chemical reaction is reduced. In other words the generation of internal heat due to exothermic chemical reaction is reduced and hence thermal stability of the system is encouraged. It should be noted that as the internal heat generation occurs with increasing time, the temperature of the system reaches a stage where no further increase takes place. This phenomenon is called steady state of the system and it is illustrated by Figures 10 - 11 where the temperature cannot increase anymore at time $t > 0$.

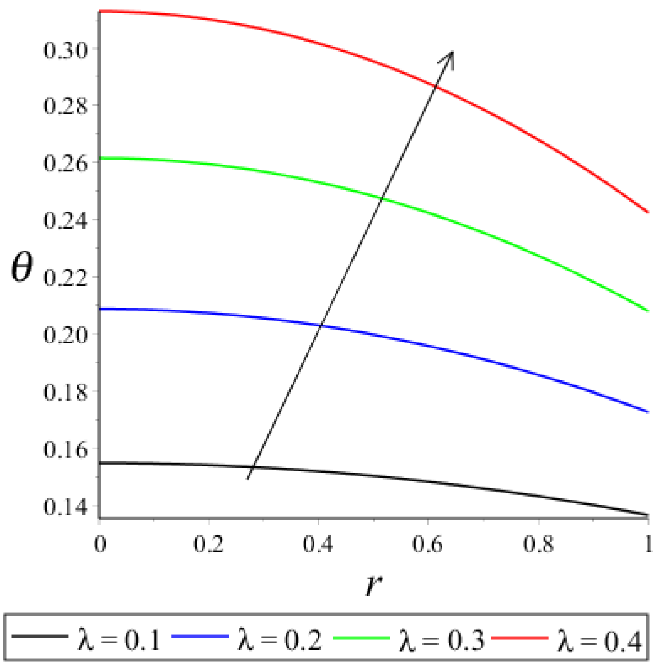

Figure 2: λ effect on temperature

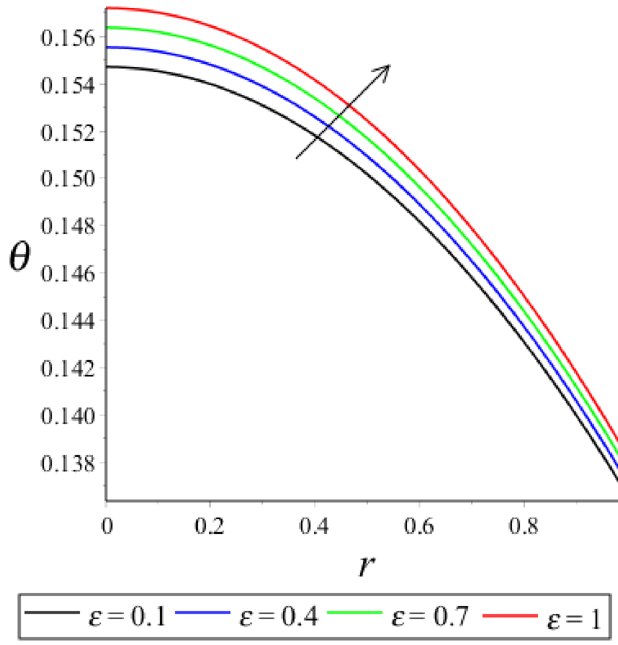

Figure 3: ε effect on temperature

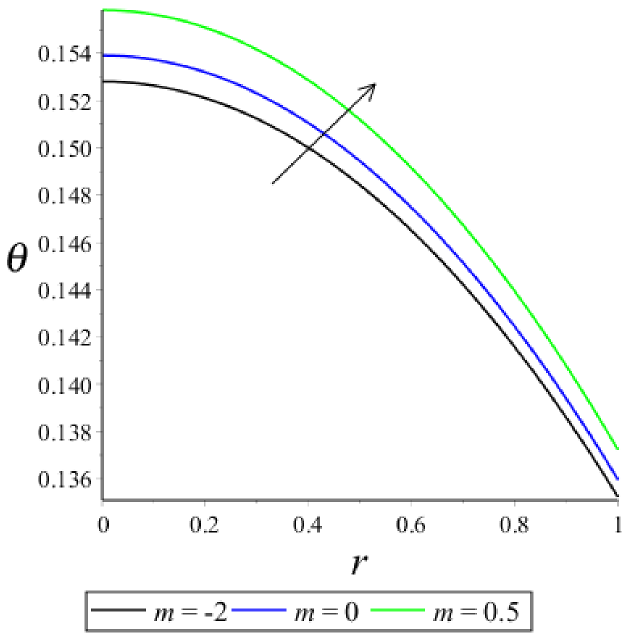

Figure 4: m effect on temperature

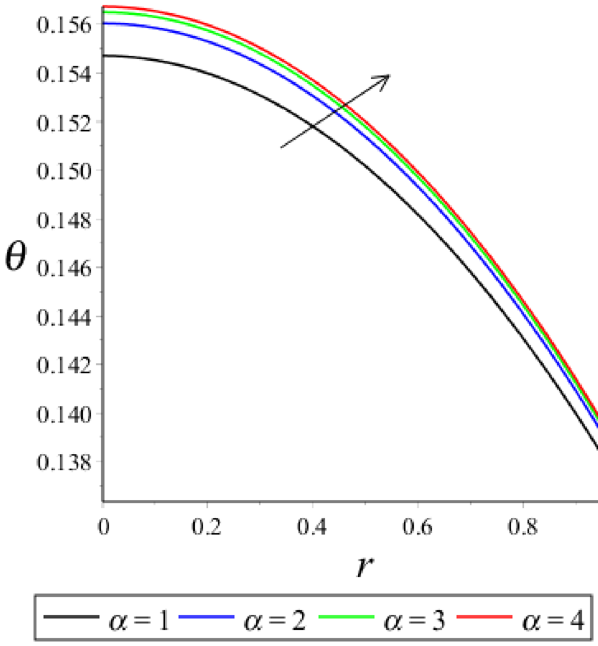

Figure 5: α effect on temperature

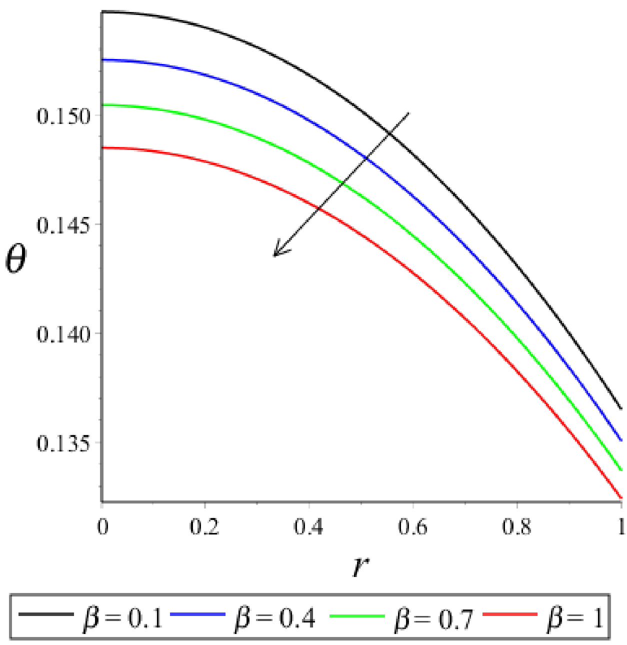

Figure 6: β effect on temperature

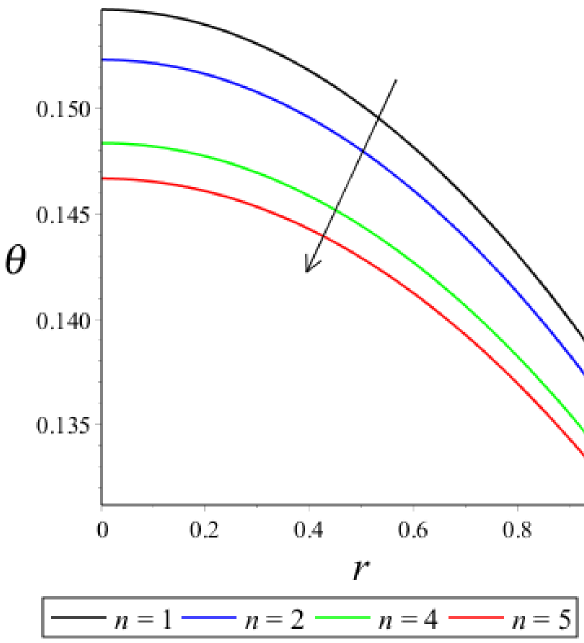

Figure 7: *n* effect on temperature

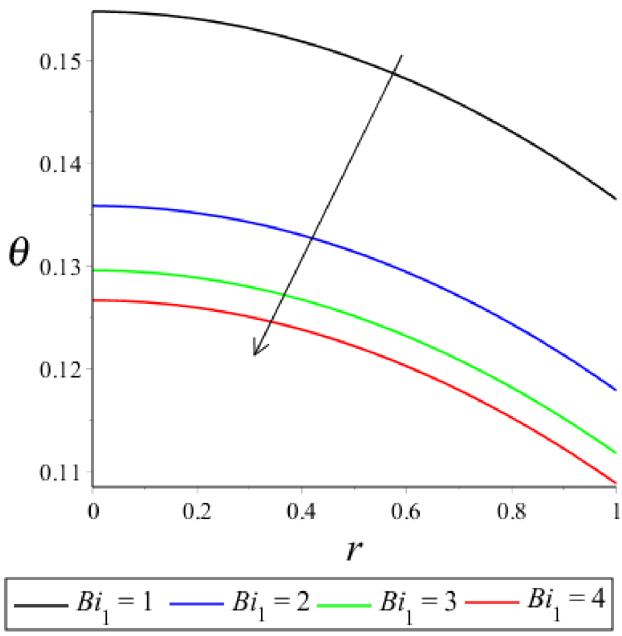

Figure 8: Bi_1 effect on temperature

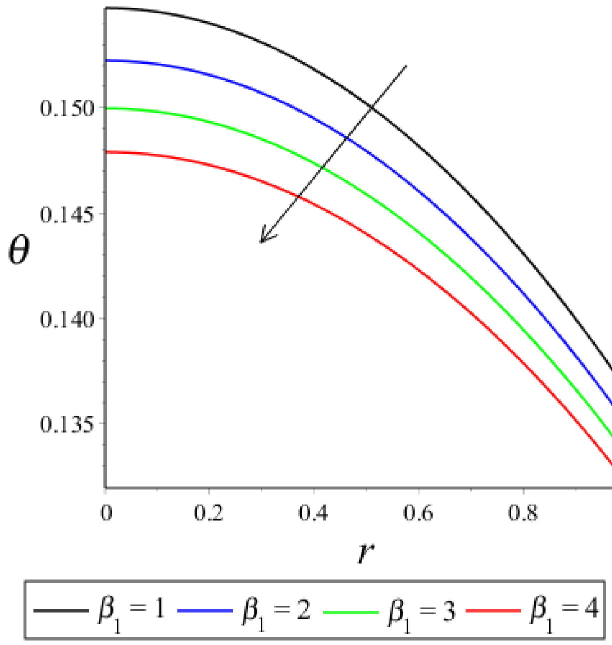

Figure 9: β_1 effect on temperature

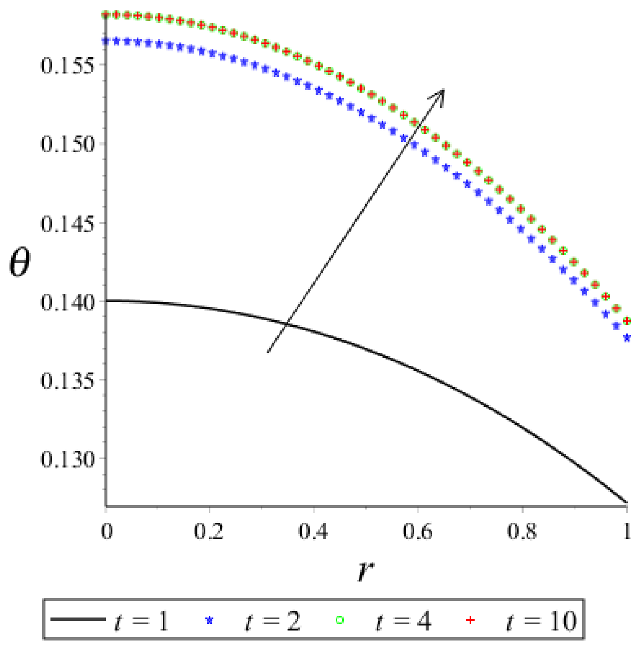

Figure 10: t effect on temperature

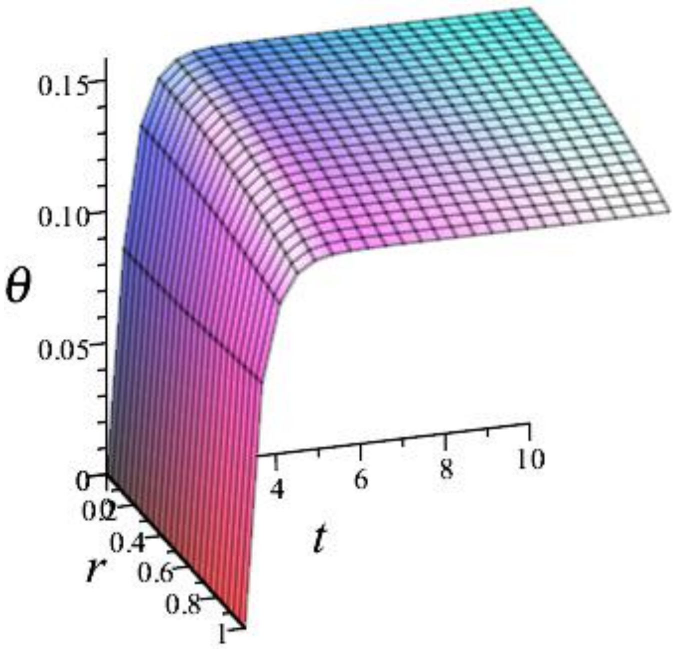

Figure 11: 3-D t effect on temperature

4.2 Effects of thermo-physical parameters on oxygen depletion

Here we consider effects of parameters on oxygen depletion. The variations of each parameter are depicted in Figures 12 – 23. A general observation is that oxygen concentration is lowest at the center of the sphere and highest at the surface. This confirms the consumption of oxygen in combustion process. Figures 12 – 16 show respectively, variations of parameters n, Bi_1, Bi_2, β and α, with their effects on oxygen depletion. We observe that an increase in these parameters result with corresponding increase in oxygen profiles. This means that oxygen depletion is reduced and oxygen concentration is retained at high values of these parameters. The significance of oxygen depletion reduction is that the exothermic chemical reaction of the system is also discouraged to perpetuate more heat generation within the system. We see a different scenario in Figures 17 – 22, where an increase in parameters m, λ, β_1 and ε, results with a decrease in oxygen profiles. These parameters encourage exothermic chemical reaction to occur and therefore more consumption rate of oxygen is experienced. Figures 22 – 23 show the effect of increased time t on oxygen depletion. We see that towards steady state attainment, oxygen profiles increase until no action takes place when steady state is achieved. This confirms that as time t increases in a combustion process, oxygen depletion tends to reduce when steady state is attained.

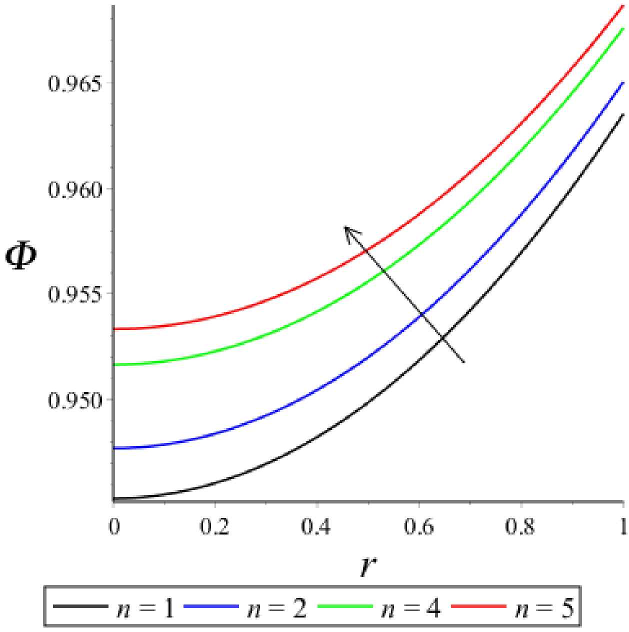

Figure 12: n effect on oxygen depletion

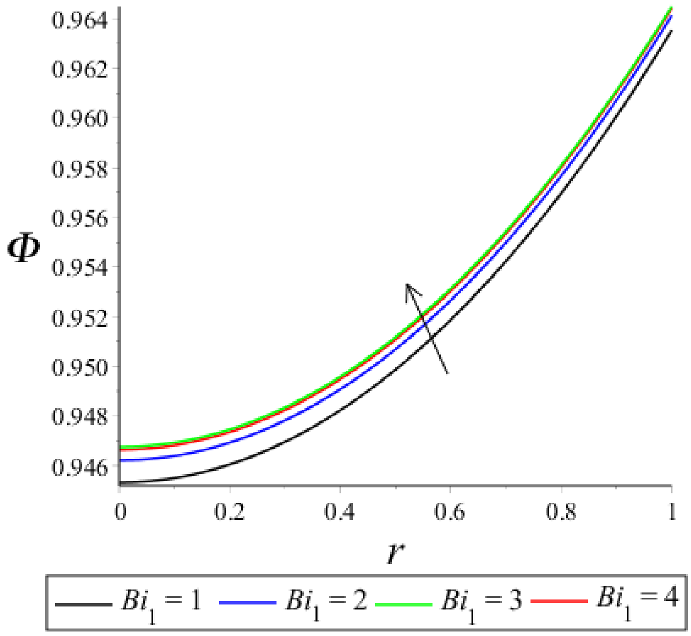

Figure 13: Bi_1 effect on oxygen depletion

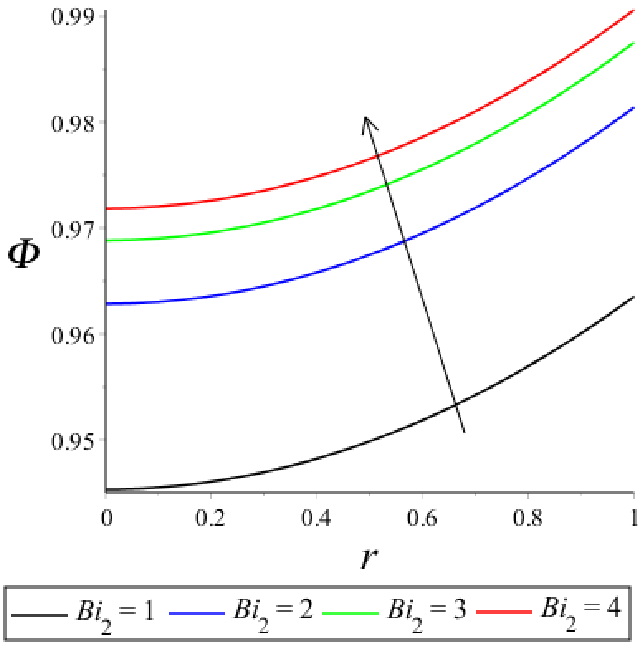

Figure 14: Bi_2 effect on oxygen depletion

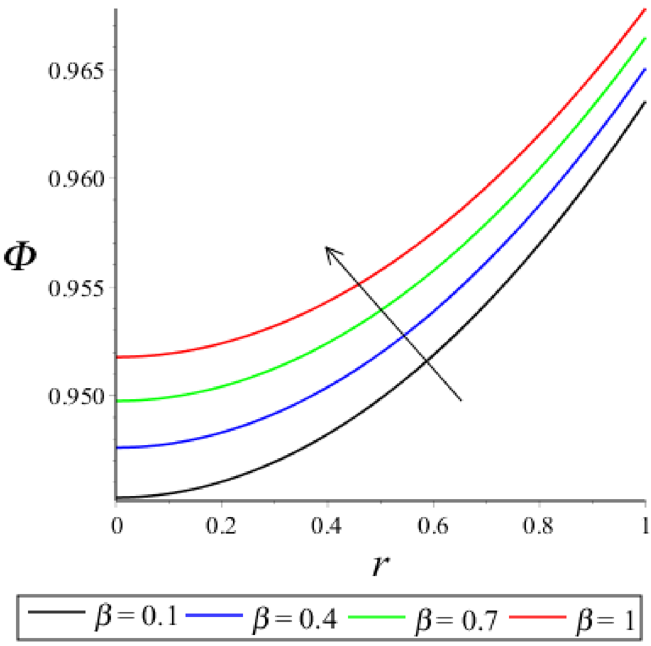

Figure 15: β effect on oxygen depletion

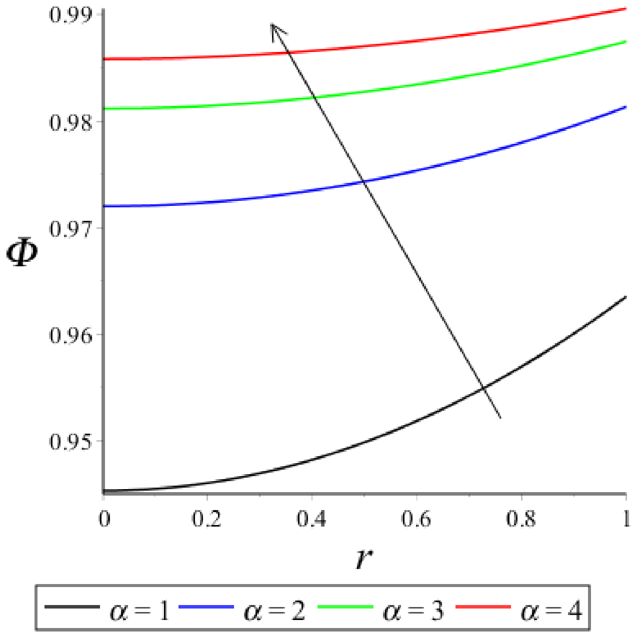

Figure 16: α effect on oxygen depletion

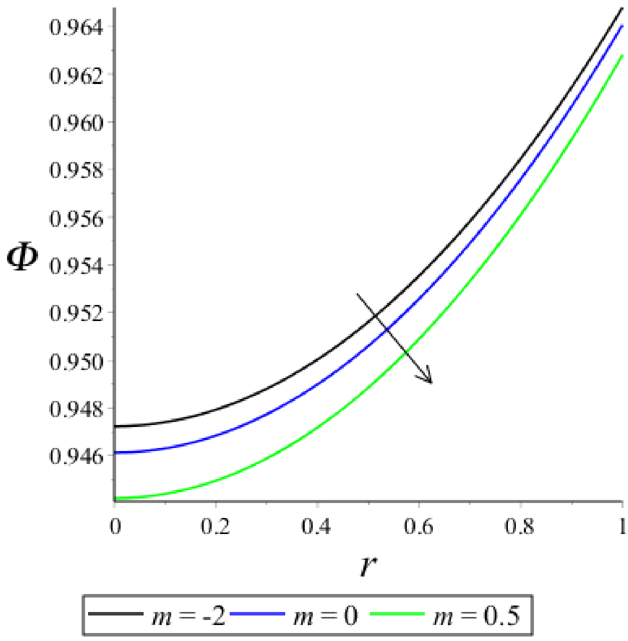

Figure 17: m effect on oxygen depletion

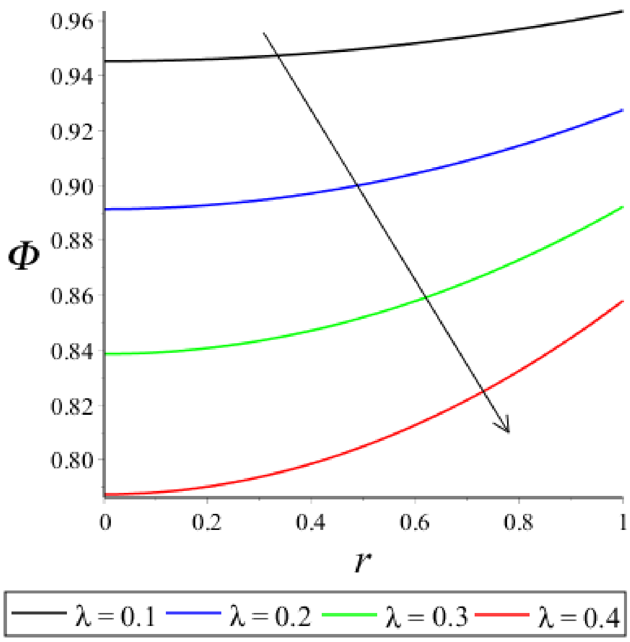

Figure 18: λ effect on oxygen depletion

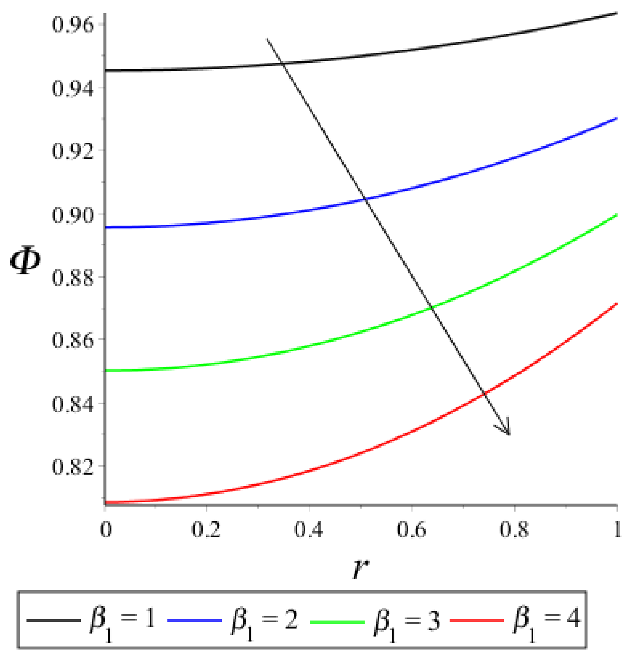

Figure 19: β_1 effect on oxygen depletion

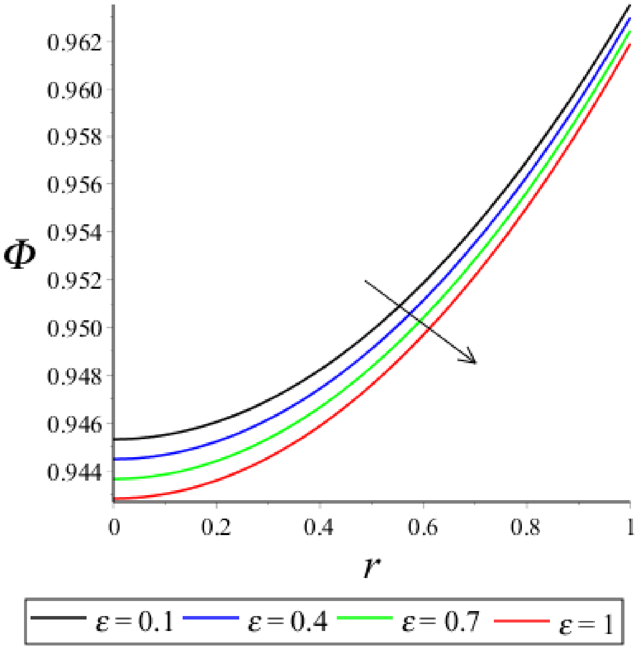

Figure 20: ε effect on oxygen depletion

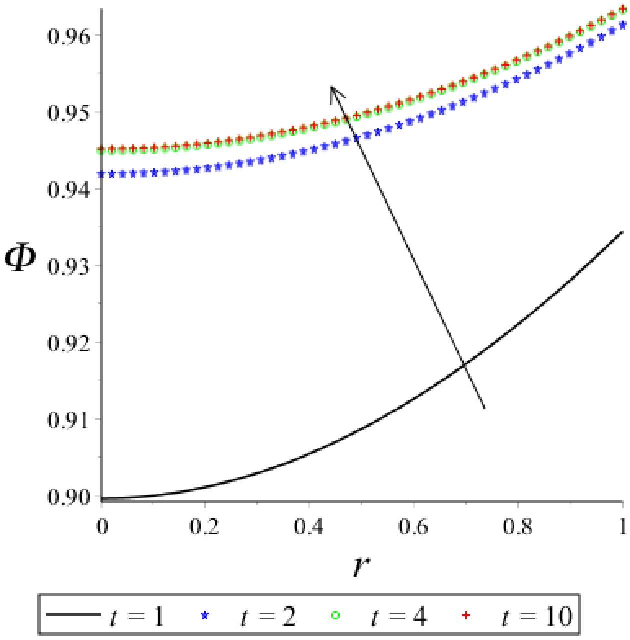

Figure 21: t effect on oxygen depletion

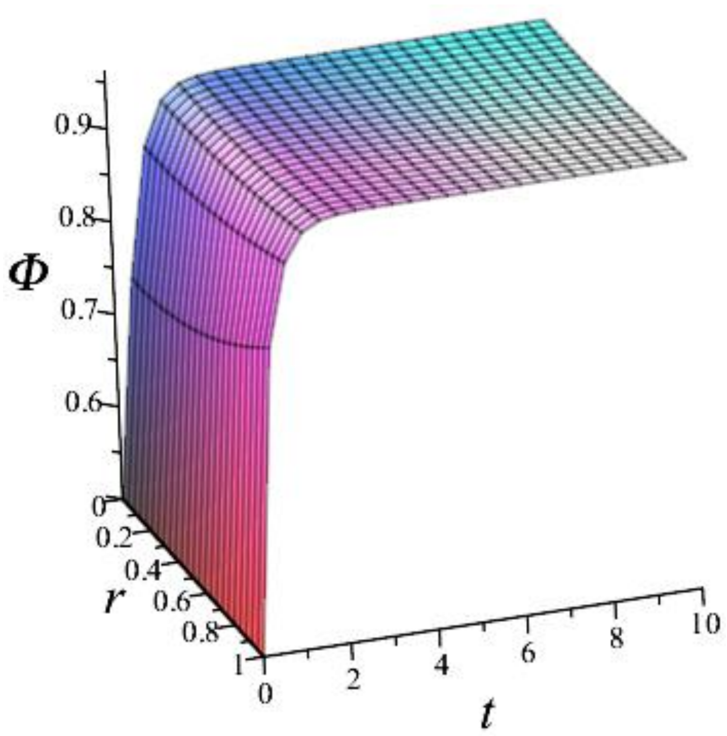

Figure 22: 3-D *t* effect on oxygen depletion

4.3. Thermal stability analysis

In this subsection we analyze thermal stability by plotting the Nusselt number (Nu) against the Frank-Kamenetskii or reaction rate parameter (λ). The results are illustrated in Figures 23 – 29 for the following parameters, $m, Bi_2, \alpha, \beta_1, n, \varepsilon,$ and Bi_1. Thermal stability is illustrated by the longest graph that corresponds to the highest value of λ. The numerical values for Nu and λ due to variation of the mentioned parameters to understand the thermal stability depicted in the graphs are given in Table 1. We observe from Figures 23 – 26 that an increase in the parameters m, Bi_2, α and β_1 results with a decrease in λ values. This means that thermal stability is attained by keeping lowest values of these parameters. A different scenario is observed in Figures 27 – 29 where an increase in $n, \varepsilon,$ and Bi_1 gives a corresponding increase in the λ values. This implies that thermal stability is attained at highest values of the parameters $n, \varepsilon,$ and Bi_1.

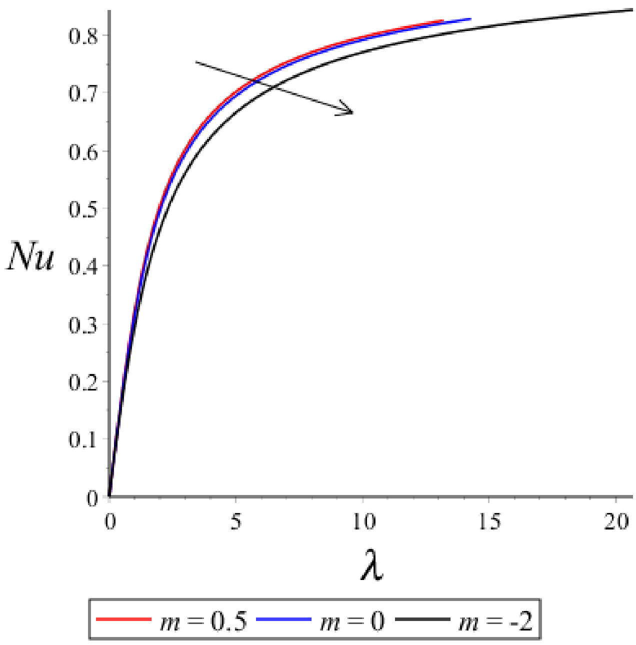

Figure 23: m effect on thermal stability

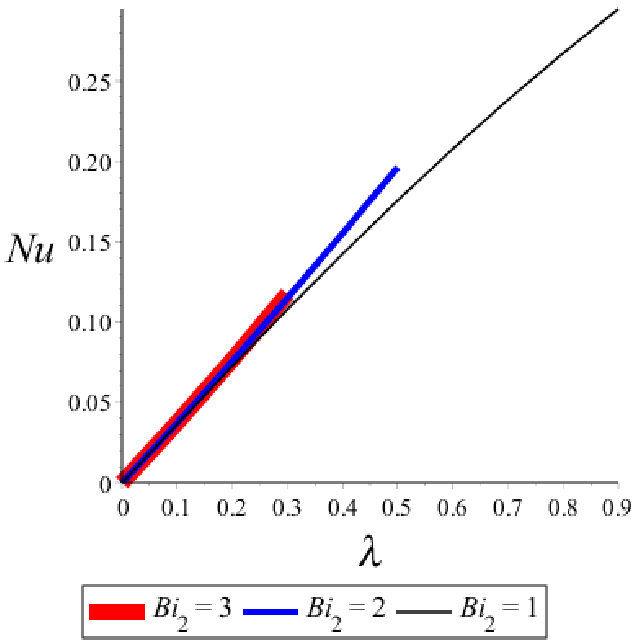

Figure 24: Bi_2 effect on thermal stability

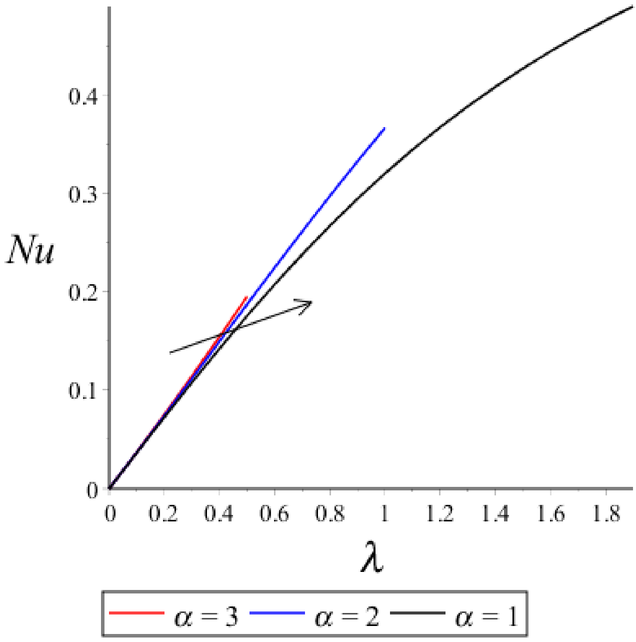

Figure 25: α effect on thermal stability

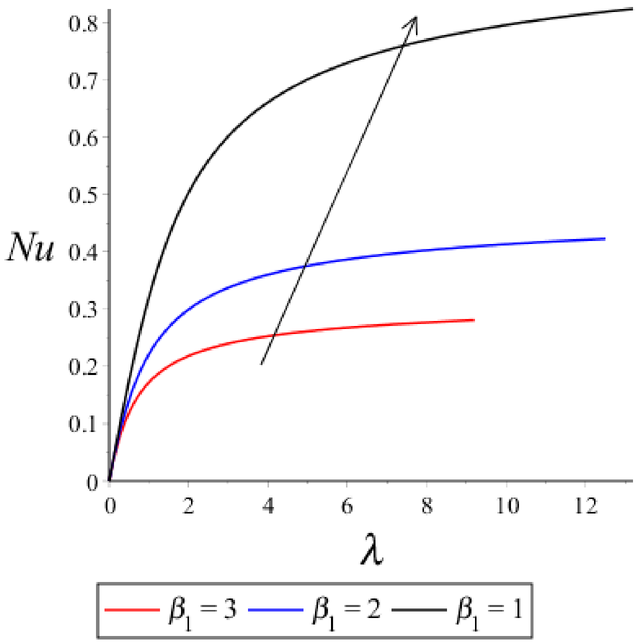

Figure 26: β_1 effect on thermal stability

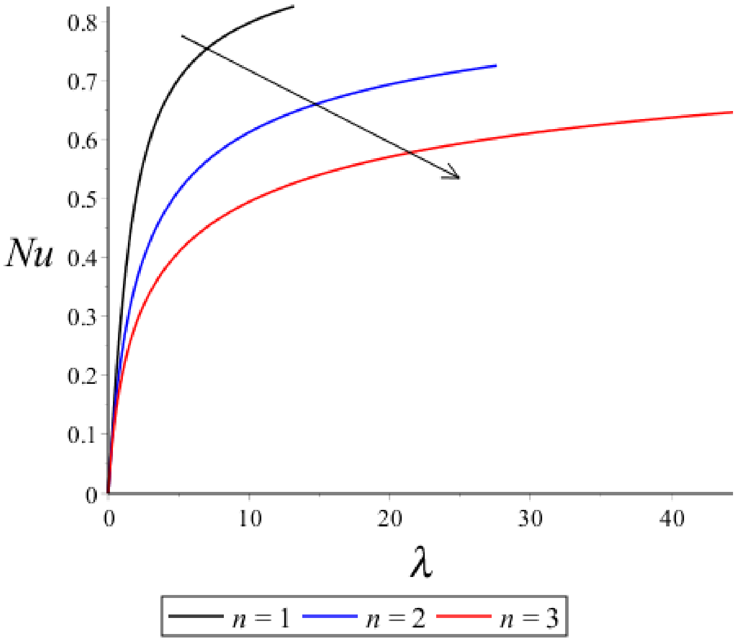

Figure 27: *n* effect on thermal stability

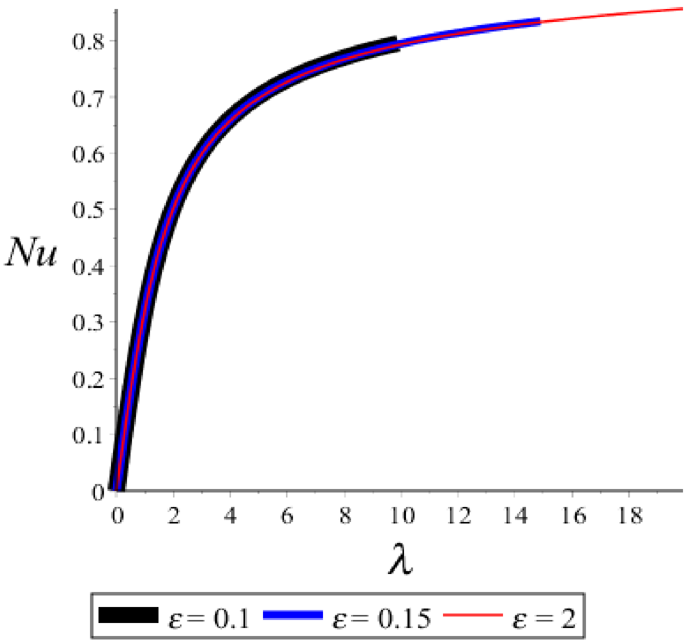

Figure 28: ε effect on thermal stability

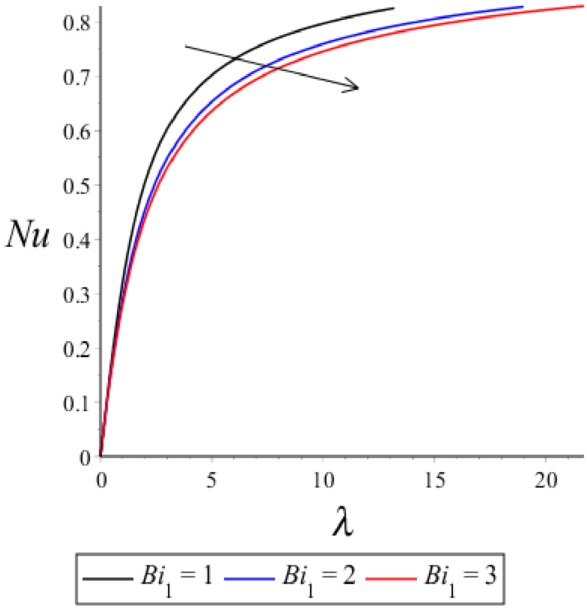

Figure 29: Bi_1 effect on thermal stability

Values obtained for Nu and λ for varied $m, Bi_2, \alpha, \beta_1, n, \varepsilon,$ and Bi_1 respectively, are given in Table 1 below.

Table 1: Numerical values showing effects of thermo-physical parameters on thermal criticality values.

m	Bi_2	α	β_1	n	ε	Bi_1	Nu	λ
-2	1	1	1	1	0.1	1	0.99529	20830.4090
0	1	1	1	1	0.1	1	0.99490	14408.5993
0.5	1	1	1	1	0.1	1	0.99484	13360.2093
0.5	2	1	1	1	0.1	1	1.28819	5.9443
0.5	3	1	1	1	0.1	1	1.60960	4.3943
0.5	1	2	1	1	0.1	1	1.30852	11.6392
0.5	1	3	1	1	0.1	1	1.51476	6.7964
0.5	1	1	2	1	0.1	1	0.49765	12607.2510
0.5	1	1	3	1	0.1	1	0.33172	9326.8513
0.5	1	1	1	2	0.1	1	0.94227	2777.8178
0.5	1	1	1	3	0.1	1	0.96470	4.457906229×10^5
0.5	1	1	1	1	0.15	1	0.99491	14045.5100
0.5	1	1	1	1	0.2	1	0.99498	14729.8091
0.5	1	1	1	1	0.1	2	0.99474	19168.2092
0.5	1	1	1	1	0.1	3	0.99471	21827.9693

5. CONCLUSION

In this article we looked at effects of various embedded thermo-physical parameters on temperature and oxygen depletion in a stockpile of reactive material modelled in a spherical domain. The sphere was assumed to be of variable thermal conductivity. It was observed that the following thermo-physical parameters, λ, ε, m and α, facilitate the exothermic chemical reaction which generates more heat in the system and thus raising the temperature levels during combustion. The parameter α increases both the levels of temperature and oxygen diffusion during combustion. The mentioned parameters also fast-trek oxygen depletion during combustion, because their effects on oxygen depletion reduce the system's oxygen concentration. A different scenario was observed for the parameters, n, Bi_1, Bi_2 and β, which help in preservation of oxygen during combustion and therefore also reducing the levels of temperature of the system. These parameters are also helpful to attain thermal stability when their values are kept very high. The approach to this investigation involved theory only. The advantage of this theoretical investigation of self-igniting processes is to provide a cheaper and simpler way of understanding factors that enhance temperature increases or oxygen depletion, by using mathematical approach. This study can be extended to a two-step combustion scenario in a reactive sphere.

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