# On Heat Transfer Analysis for a Sphere of Combustible Material of Variable Thermal Conductivity

**Ramoshweu Solomon Lebelo[1, a\*], Radley Kebarapetse Mahlobo[1, b], Samuel Olumide Adesanya[1, 2, c], Mohana Sundaram Muthuvalu[3, d]**

[1]Vaal University of Technology, Mathematics Department, Andries Potgieter Blvd, Vanderbijlpark, 1911, South Africa
[2]Redeemer's University, Mathematical Sciences Department, PMB 230 Ede, Osun State, Nigeria.
[3]Universiti Teknologi PETRONAS, Fundamental and Applied Sciences Department, 32610 Seri Iskandar, Perak Darul Ridzuan, Malaysia.

[a\*]sollyl@vut.ac.za, [b]radley@vut.ac.za, [c]adesanyas@run.edu.ng, [d]mohana.muthuvalu@petronas.com.my

**Abstract.** This article considers an exothermic chemical reaction taking place in a stockpile of reactive material with a thermal conductivity that is temperature dependent. The study is modeled in a spherical domain whose carbon-containing material reacts spontaneously with the oxygen trapped within the system. The combustion process results with a complicated process that is nonlinear in nature, and the energy equation used to govern the problem is tackled numerically with the semi-implicit finite difference method (FDM). The results are depicted graphically and discussed to give a theoretical understanding of the heat transfer analysis during combustion.
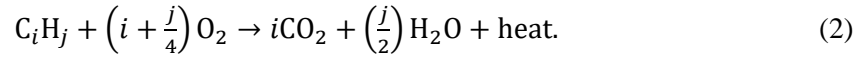
## 1. Introduction

Exothermic chemical reaction in combustible materials has drawn a lot of research because of spontaneous reaction that takes place within a stockpile of such materials. Most of the veld fires that are hazardous to live species are caused by spontaneous combustion taking place within stockpiles of combustible materials such as coal, hay, wood, wool or any dumbed rubbish in the open space [1, 2]. Spontaneous ignition is due to the readiness of the carbon-containing material to react with the oxygen trapped within the material when the exothermic chemical reaction takes place [3]. The process of combustion gives heat as one of the products, and this generated heat raises the temperature of the system. Progressive generation of heat rate should not exceed its rate of release to the surrounding environment, because this situation leads to thermal runaway that breeds self-ignition [4-6]. It is known that heat transfer involves energy transport due to conduction, convection and radiation, but in this study, we assume convection as the only means of energy transport. The analysis of heat transfer in this case is done theoretically using mathematical approach that involves computer programing. This approach, requires thorough understanding of the thermo-physical parameters embedded on the partial differential equation governing the problem. The studies of heat transfer in a spherical domain were done in [7, 8] but in these cases, constant thermal conductivity was assumed. In this case, we consider thermal conductivity that is temperature depended. Variable thermal conductivity's influence on thermal ignition was studied in [9, 10], where it is clarified that the thermal conductivity varies with temperature, exponentially, as according the following equation

$$k = \mu e^{b(T-T_w)}, \tag{1}$$

where $\mu$ is the thermal conductivity of the material at the ambient temperature $T_w$, $b$ is the parameter for the variation of the thermal conductivity, and $T$ is the absolute temperature of the sphere.

The combustion process is simplified by assuming a one-step irreversible chemical kinetics expressed as [2, 8]

$$C_iH_j + \left(i + \frac{j}{4}\right)O_2 \rightarrow iCO_2 + \left(\frac{j}{2}\right)H_2O + \text{heat}. \tag{2}$$

In this analysis, it is assumed that heat generation within the combusting material follows Arrhenius law of kinetics and that this generated heat does not depend on the diffusion of the reactant, in other words, the reactant consumption is neglected. The results are graphically expressed and thoroughly discussed.

## 2. Mathematical modeling

The spherical domain of combustible material is assumed to undergo an nth order chemical kinetics. The convective heat loss to the environment obeys Newton's law of cooling, and it is described by $-\frac{h}{k}[T - T_w]$. $h$, in this case, represents the heat transfer coefficient and, $k$ the variable thermal conductivity of the material described in equation 1. The negative sign indicates the heat loss from the sphere to the surrounding environment. Figure 1 below illustrates the geometry of the problem.
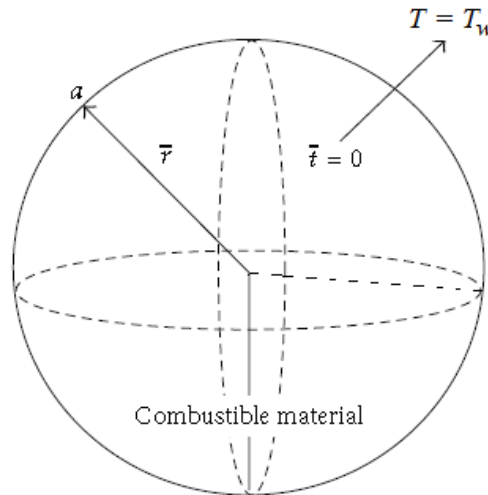


**Figure 1.** The geometry of the problem.

The following nonlinear partial differential equation in one dimension, governing the problem is given as [7, 8].

$$pc_p \frac{\partial T}{\partial \bar{t}} = k\left(\frac{\partial^2 T}{\partial \bar{r}^2} + \frac{2}{\bar{r}}\frac{\partial T}{\partial \bar{r}}\right) + QAC\left(\frac{KT}{vl}\right)^m e^{-E/RT} - \sigma(T - T_w). \tag{3}$$

Convective boundary conditions are as follows:

$$\frac{\partial T}{\partial \bar{r}}(0, \bar{t}) = 0, \tag{4}$$

$$\frac{\partial T}{\partial \bar{r}}(a, \bar{t}) = -\frac{h}{k}[T(a, \bar{t}) - T_w]. \tag{5}$$

The initial condition is

$$T(\bar{r}, 0) = T_0. \tag{6}$$

Here, $T_0$ is the initial temperature of the sphere, $\rho$ is the density, $c_p$ is the specific heat at constant pressure, $Q$ is the heat of reaction, $A$ is the rate constant and $C$ is the reactant concentration. We have $K$ as the Boltzmann's constant, $v$ as the vibration frequency, $l$ as the Planck's number, $E$ as the activation

energy and $R$ as the universal gas number. Moreover, $m$ is the numerical exponent and takes the following values, -2 for sensitized, 0 for Arrhenius and 0.5 for bimolecular kinetics. Lastly, $\bar{r}$ is the radial length of the sphere, and $\sigma$ is the heat loss parameter. The following dimensionless parameters were introduced to equation 3-6,

$$\left.\begin{array}{c} \theta = \frac{E(T-T_w)}{RT_w^2}, \theta_0 = \frac{E(T_0-T_w)}{RT_w^2}, \; Bi = \frac{ah}{k}, \\[2mm] \beta = \frac{bRT_w^2}{E}, \; \alpha = \frac{\sigma a^2}{\mu}, \\[2mm] \delta = \left(\frac{KT_\infty}{vl}\right)^m \frac{QAEa^2C}{\tau RT_\infty^2} exp\left(-\frac{E}{RT_\infty}\right), \\[2mm] r = \frac{\bar{r}}{a}, \;\; \varepsilon = \frac{RT_w}{E}, \; t = \frac{\mu\bar{t}}{\rho c_p a^2}, \end{array}\right\} \tag{7}$$

to have the following dimensionless governing equation:

$$\frac{\partial\theta}{\partial t}e^{-\beta\theta} = \frac{\partial^2\theta}{\partial r^2} + \frac{2}{r}\frac{\partial\theta}{\partial r} + \beta\left(\frac{\partial\theta}{\partial r}\right)^2 + \delta(1+\varepsilon\theta)^m e^{\theta/(1+\varepsilon\theta)}e^{-\beta\theta} - \alpha\theta e^{-\beta\theta}. \tag{8}$$

The initial condition is

$$\theta(r,0) = \theta_0, \tag{9}$$

and boundary conditions are

$$\frac{\partial\theta}{\partial r}(0,t) = 0; \tag{10}$$

$$\frac{\partial\theta}{\partial r}(1,t) = -Bi\theta e^{-\beta\theta}. \tag{11}$$

Here, $\theta$ is the dimensionless temperature, $\theta_0$ is the dimensionless initial temperature, $\delta$ is the Frank-Kamenetskii parameter also called the rate of reaction parameter, $\varepsilon$ is the activation energy parameter, $r$ is the dimensionless radial length of the sphere, and $\beta$ represents the dimensionless variable thermal conductivity parameter. $Bi$ is the thermal Biot number at the surface of the sphere, and $\alpha$ is the dimensionless heat loss parameter. The dimensionless heat transfer rate at the surface of the sphere is described by $Nu = -\frac{d\theta}{dy}$, called the Nusselt number ($N$).

## 3. Numerical approach
The application of the semi-implicit finite difference scheme involves taking implicit terms at intermediate time level ($N + \xi$) for $0 \leq \xi \leq 1$. For this study, $\xi = 1$ was used to enable use of larger time steps for convenience. The approximation of the partial differential equation that governs the problem, was done at the second-order central differences. The boundary conditions were obtained from the modification of the equations that corresponded to the first and the last grid points, and the finite differences for the discretization of the governing equation are taken from the linear Cartesian mesh and uniform grids. The semi-implicit FDM for the governing equation is ultimately expressed as:

$$\left(\frac{\theta^{N+1}-\theta^N}{\Delta t}\right)e^{-\beta\theta} = \frac{\partial^2}{\partial r^2}\theta^{N+\xi} + \frac{2}{r}\frac{\partial}{\partial r}\theta^N + \beta\left(\frac{\partial}{\partial r}\theta^N\right)^2 - \alpha\left(\theta e^{-\beta\theta}\right)^N +$$
$$\delta\left[(1+\varepsilon\theta)^m\Phi^n e^{\left(\frac{\theta}{1+\varepsilon\theta}\right)}e^{-\beta\theta}\right]^N \tag{12}$$

The unknown new time ($N + 1$) terms are placed on the left, whilst the known terms at the present time ($N$) are placed on the right side of the equation. The following expression is attained,

$$-\xi\tau\theta_{j+1}^{N+1} + \left(e^{-\beta\theta} + 2\xi\tau\right)\theta_j^{N+1} - \xi\tau\theta_{j-1}^{N+1} = -\tau(1-\xi)\theta_{j+1}^N - \alpha\Delta t\theta_{j+1}^N$$

$$+\left[e^{-\beta\theta} - 2\tau(1-\xi)\right]\theta_j^N - \frac{\Delta t\beta}{4}\left[\left(\theta_{j+1}^N - \theta_{j-1}^N\right)\right]^2 + \tau(1-\xi)\theta_{j-1}^N + \frac{1}{2r_j^2}\tau\left(\theta_{j+1}^N - \theta_{j-1}^N\right)$$

$$+ \delta\Delta t\left[(1+\varepsilon\theta)^m\Phi^n e^{\left(\frac{\theta}{1+\varepsilon\theta}\right)}e^{-\beta\theta}\right]^N \tag{13}$$

where, $j$ represents the position, $N$ the time, $\Delta r$ the mesh spacing and $\tau = \frac{\Delta t}{\Delta r^2}$ equation 13 forms a tri-diagonal system that was solved using MAPLE in this study. Graphical solutions to understand the temperature behavior during combustion are presented in the following section.

**4. Results and discussion**.
In this section, results are graphically presented and discussed. Unless or otherwise stated, the following parameters were applied

$$\beta = 1, \delta = 0.1, \alpha = 1, \varepsilon = 0.1, m = 0.5, Bi = 1, t = 10.$$

*4.1. Steady state temperature profiles*
The steady state is attained when the temperature of the system is no more dependent on the time. This is illustrated in figure 2 and figure 3, where at some time $t > 0$, the temperature of the system remains constant. It is observed that the temperature profiles are high at the center of the sphere, due to continued exothermic chemical reaction within the sphere. The exothermic chemical reaction produces heat as one of the products of combustion and this results with high profiles of temperature. The profiles of temperature drop toward the surface of the sphere because of progressive heat loss due to convection at the surface of the sphere.
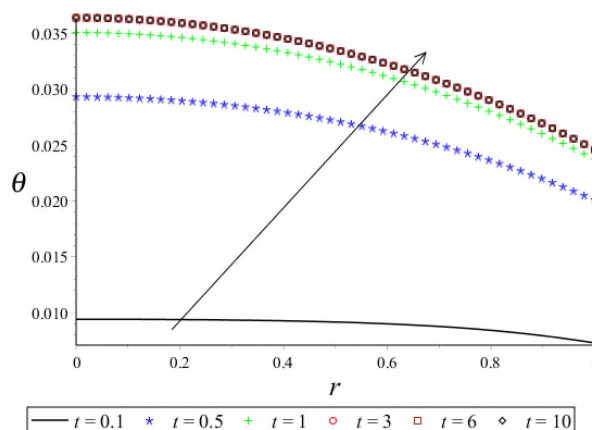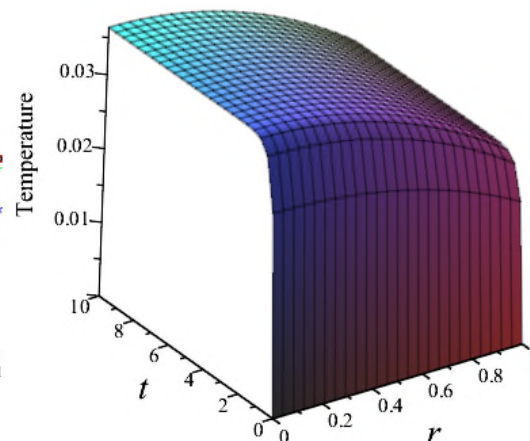


**Figure 2.** 2-D Steady state.              **Figure 3**. 3-D Steady state.

*4.2. Unsteady state temperature profiles*
In this subsection, we consider the influence of the variation of selected kinetic parameters on the heat transfer process, hence the temperature behavior of the system. The following parameters $\delta, \varepsilon, \beta, m, \alpha$ and $Bi$ were each varied, while others kept constant, to investigate the heat transfer. The figure 4-9 show the behavior of the temperature due the influence of all the stated parameters, as they are respectively presented. We see from figure 4-7 that a combined increase in the parameters $\delta$ (reaction rate), $\varepsilon$ (activation energy), $\beta$ (variable thermal conductivity) and $m$ (chemical kinetics index) gives an increase in the temperature profiles. The increase in $\delta$ accelerates the rate of the exothermic chemical reaction to generate more heat. The same is observed with an increase in $\varepsilon$, to indicate that at higher levels of the activation energy, the exothermic chemical reaction is accelerated. The increase in $\beta$ confirms the

dependence of the thermal conductivity on the temperature of the system. It is of interest to note that the exothermic chemical reaction is fastest, during bimolecular kinetics ($m = 0.5$), hence highest temperature profile, compared to Arrhenius kinetics ($m = 0$). The exothermic chemical reaction is very slow during sensitized kinetics ($m = -2$), as indicated by the lowest temperature profile.
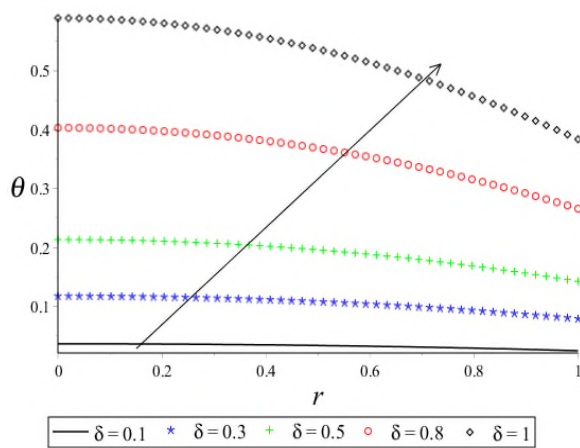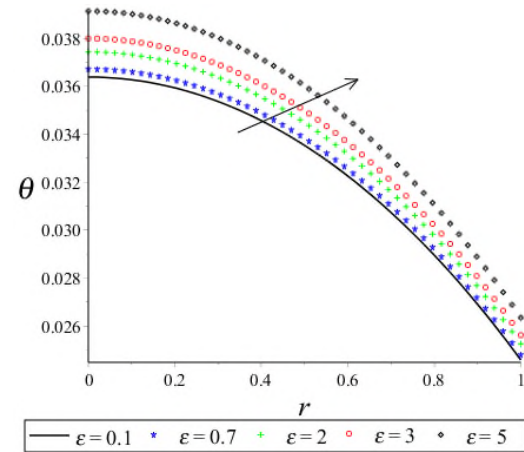


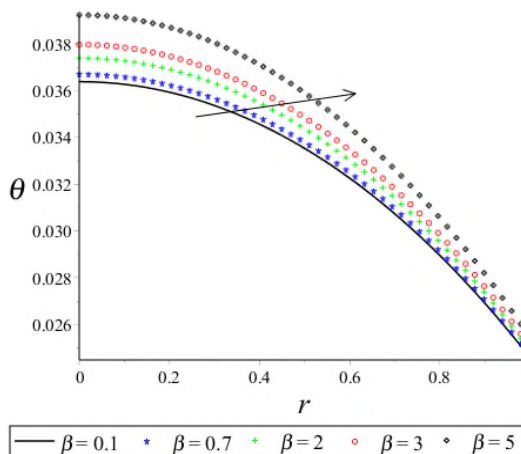**Figure 4.** δ on temperature.



**Figure 5.** ε on temperature.



**Figure 6.** β on temperature.
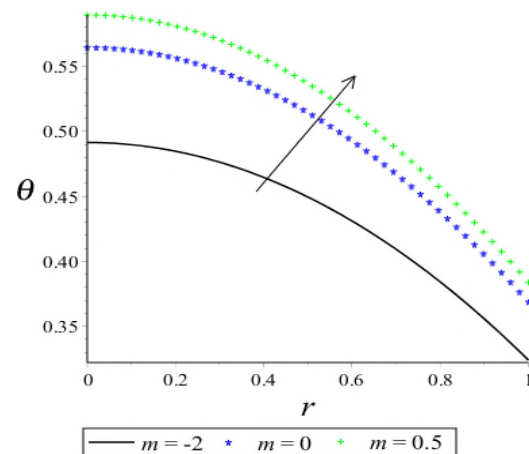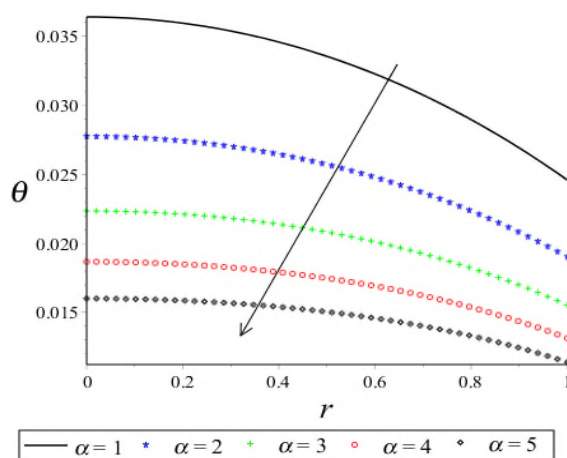


**Figure 7**. $m$ on temperature.



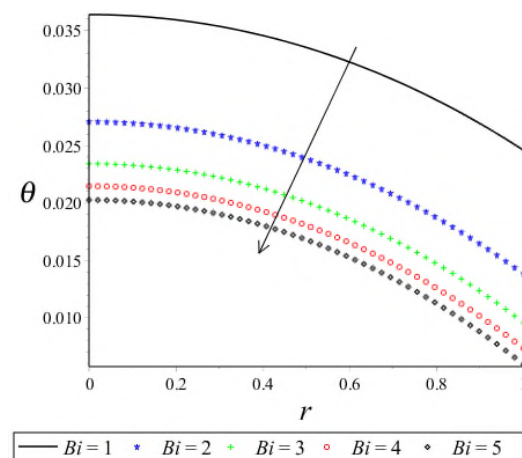**Figure 8.** $\alpha$ on temperature.



**Figure 9**. $Bi$ on temperature.

Contrary to what has happened, we observe that a combined increment in the parameters $\alpha$ (heat loss) and $Bi$ (temperature biot number) results with a decline in the temperature profiles, as illustrated in figure 8, 9. An increase in $\alpha$ means that the rate of heat loss at the surface of the sphere is increased, hence the temperature of the system's reduction. The same is observed with the increase in $Bi$, that there is a decline in the temperature of the system. This is due to increased rate of heat loss due to convection at the surface of the sphere. The last two parameters are good for discouraging the exothermic chemical reaction from taking place to control self-ignited fires.

## 5. Conclusion

The analysis of heat transfer in a combusting stockpile of reactive materials modeled in a spherical domain of variable thermal conductivity was presented in this article. It was discovered that some parameters encourage exothermic chemical reaction, whilst others discourage the reaction from taking place in stockpiles of combustible materials. The parameters $\delta, \varepsilon, \beta, \alpha$ and, $m$ were found to favor the taking place of the exothermic chemical reaction. The occurrence of the exothermic chemical reaction releases more heat into the combusting sphere, and the accumulation of heat causes the raising up of the temperature gradient during combustion. It is better to keep these parameters very low to reduce self-ignition process in stockpiles of combustible materials. On the other hand, it was found out that the parameters $\alpha$ and $Bi$ favor the reduction of the temperature during the combustion. These parameters should be kept high to avoid self-ignited fires from explosions. This study was done theoretically to make the understanding of the combustion process in a cheaper and a quicker way compared to the experimental one. The understanding of the imbedded parameters on heat transfer can help in the control of self-ignition process in the storage of reactive materials. This study can be extended to two-step exothermic chemical reaction processes.

## 6. References

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