On transient heat analysis of a two-step convective reactive cylinder

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Abstract. This article looks at the analysis of heat transfer due to combustion of reactive materials in a stockpile modelled in a cylindrical domain. The transient heat analysis is studied through the investigation of effects kinetic parameters, embedded on the differential equation governing the problem, have on the temperature of the system. The temperature patterns due to the parameters effect, are depicted in graphs generated through Maple software. The complicated nonlinear partial differential equation is solved numerically using Finite difference method (FDM). The results show that parameters such as the order of reaction slow down the exothermic chemical reaction, while parameters like the reaction rate enhance the combustion process.

Introduction

The study of combustion in reactive materials due to exothermic chemical reaction has drawn the attention of many researchers. This is due to spontaneous combustion taking place in stockpiles of coal, hay, wood, wool or dumbed rubbish in the open veld, for example. The literature shows that some of veld fires are caused by spontaneous combustion when the carbon containing material reacts readily with the oxygen trapped within the stockpile [1,2]. Heat is one product of combustion, and the transfer of heat in reactive materials has many industrial applications. Some of the applications include, among others, the combustion process design inside engines and exhaust systems of automobiles, solids combustion, the heavy oil recovery process, cellulose material storage and waste material incineration [3,4,5]. It is also important to note that ignorance of heat transfer knowledge in industrial products manufacturing is the reason behind decolorization and bending of such products [6]. Experimental studies on spontaneous combustion of reactive materials in stockpiles were investigated in [7,8,9], where parameters such as the ambient temperature, material’s coarseness and humidity of the material, for example, were considered. In this study, a theoretical approach to combustion process analysis is conducted, where the process is made easy to understand by considering the behaviour patterns of the temperature subjected to variations of selected parameters embedded on the governing differential equation, as investigated in [10,11,12]. Two-step exothermic chemical reaction was studied in [13,14] in a reactive slab, and modelling in a cylinder and sphere was conducted respectively in [15,16]. In this investigation, focus is on heat loss to the ambient by convection only.
Mathematical Formulation

An $n^{th}$ order exothermic chemical reaction in a stockpile of reactive materials with constant thermal conductivity $k$ is assumed. An example of a two-step reaction mechanism is that of methane combustion in air:

\[ 2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O \]  \hspace{1cm} (1)

\[ 2CO + O_2 + H_2O \rightarrow 2CO_2 + H_2O \]  \hspace{1cm} (2)

Heat loss to the ambient by convection obeys Newton's law of cooling and it is expressed by

\[-\frac{h}{k}[T - T_b] , \]

where $h$ is the heat transfer coefficient, $k$ is the thermal conductivity of the material, $T$ is the absolute temperature of the cylinder, and $T_b$ is the ambient temperature. The geometry of the problem is illustrated in figure 1 below.

\[ \begin{align*}
\text{Convective heat loss} & \hspace{1cm} \hat{r} = a \\
\text{Combustible material} & \hspace{1cm} \hat{r} = 0 \\
& \hspace{1cm} x
\end{align*} \]

**Figure 1.** Geometry of the problem

The energy equation for combustion process in the two-step exothermic chemical reaction, is expressed by [10]

\[ p c_p \frac{\partial T}{\partial t} = \frac{k}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + Q_1 A_1 C_1 \left( \frac{k T}{v l} \right)^m e^{-E_1/RT} + Q_2 A_2 C_2 \left( \frac{k T}{v l} \right)^m e^{-E_2/RT} . \]  \hspace{1cm} (3)

The boundary and initial conditions are respectively

\[ \frac{\partial T}{\partial r} (0, \ell) = 0; \quad \frac{\partial T}{\partial r} (a, \ell) = -\frac{h}{k} (T - T_b); \quad T(\ell, 0) = T_0 \]  \hspace{1cm} (4)

$T_0$ represents the cylinder initial temperature, $Q_1$, $A_1$ and $C_1$ respectively, are the first step heat of reaction, rate constant, and reactant’s concentration, and, $Q_2$, $A_2$ and $C_2$, are respectively, the second step’s heat of reaction, rate constant, and reactant’s concentration. The activation energies for the first and second steps respectively are $E_1$ and $E_2$. The chemical kinetics type is represented by $m$, $m = -2$ represents the light induced kinetics, $m = 0$ the Arrhenius kinetics, and $m = 0.5$ the bimolecular kinetics.

Dimensionless parameters are introduced in this manner

\[ \theta = \frac{E_1 (T - T_b)}{RT_b}, \theta_0 = \frac{E_1 (T_0 - T_b)}{RT_b}, r = \frac{r}{a}, \varepsilon = \frac{RT_b}{E_1}, \varepsilon = \frac{E_2}{E_1}, t = \frac{t}{a \sqrt{\varepsilon}}, B = \frac{ah}{k} \]

\[ \omega = \frac{Q_2 A_2 E_2}{Q_1 A_1 E_0} e^{(E_1 - E_2)/RT}, \alpha = \left( \frac{k T_b}{v l} \right)^m \frac{Q_0 A_1 a^2 C_1}{k R T_b} e^{-E_1/RT} . \]  \hspace{1cm} (5)

It follows that equations (3) – (4) take the following forms:

\[ \frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r} + \alpha (1 + \varepsilon \theta)^m e^{[\theta/(1 + \varepsilon \theta)]} + \alpha \omega (1 + \varepsilon \theta)^m e^{[\theta/(1 + \varepsilon \theta)]} . \]  \hspace{1cm} (6)

The boundary and initial conditions are

\[ \frac{\partial \theta}{\partial r} (0, t) = 0; \quad \frac{\partial \theta}{\partial r} (1, t) = -B [\theta (1, t) - \theta_b], \quad \theta (r, 0) = \theta_0 \]  \hspace{1cm} (7)

where $\theta$ is the dimensionless temperature, $\theta_0$ is the dimensionless initial temperature, $\theta_b$ is the dimensionless ambient temperature, $B$ is the Biot number, $\alpha$ is the Frank-Kamenetskii parameter
(reaction rate parameter), $\varepsilon$ is the dimensionless activation energy parameter, $r$ is the dimensionless radial distance, $\varepsilon$ is the activation energy ratio parameter, $\omega$ is the two-step exothermic chemical reaction parameter.

**Numerical Approach**

The governing equation is discretized based on a linear Cartesian mesh with uniform grid to obtain finite differences. The intermediate time level given by $(N + \xi)$ with $0 \leq \xi \leq 1$, helps to determine the implicit terms. $\xi = 1$ is applied for use of larger time steps, to allow any value of the time step. The algorithm to solve the governing equation is embedded in any numerical computer software, and in this case, Maple was used.

**Results and Discussion**

Figures 2 to 6 indicate effects of parameters $\alpha$ (rate reaction), $\varepsilon$ (activation energy), $m$ (kinetic type), $\omega$ (two-step exothermic chemical reaction) and $B$ (Biot number) on the temperature of the system. An increase in the temperature is observed from figures 2 – 5, when the parameters $\alpha$, $\varepsilon$, $m$ and $\omega$ become large. These parameters enhance the exothermic chemical reaction to accelerate the combustion process, and continued combustion produces heat accumulation within the stockpile, hence the elevation of the system temperature. From figure 3, it is noticed that the exothermic chemical reaction is fastest in the bimolecular kinetics ($m = 0.5$) followed by the Arrhenius kinetics ($m = 0$), and slow in the light induced kinetics ($m = -2$). For environmental purposes, it is better to slow down the emission of heat from combustion, and this can be achieved by retardation of the exothermic chemical reaction. Fortunately, the parameter $B$ in figure 6 shows a decline in the temperature as the parameter value is increased. This means that an increase in the rate of heat release at the surface of the matter during combustion, slows down the exothermic chemical reaction to a point where the combustion may cease to take place. When combustion of the material diminishes, the heat transfer to the ambient also reduces and this is valuable for lessening global warming and climate change.

![Figure 2. Effects of $\alpha$](image1)

![Figure 3. Effects of $\varepsilon$](image2)

![Figure 4. Effects of $m$](image3)
Conclusion
In this article, analysis of combustion in a two-step exothermic chemical reaction in a stockpile of reactive materials modelled in a cylindrical domain was conducted. The study was done theoretically by applying mathematical modelling to simplify the complicated process of combustion, to enable the understanding of heat transfer in a cheaper and quicker manner. Maple Software was used to plot graphical results. From the results obtained, it was observed that the parameters $\alpha$ (rate reaction), $\varepsilon$ (activation energy), $m$ (kinetic type), and $\omega$ (two-step exothermic chemical reaction) enhance the combustion process because the temperature of the system is increased with an increase in the values of these parameters. This has adverse consequences for the environment because continued release of heat during combustion contributes to global warming and climate change. The opposite observation was illustrated by the parameter $B$ (Biot number), which slows down the exothermic chemical reaction to minimize the combustion process. This study can be extended to a combustion process where thermal conductivity of the combustible material is temperature dependent.

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