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Steady-state heat transit investigation in a radiative cylindrical pipe of reactive materials

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Abstract: This study investigates heat transfer in a combustible material modeled within a cylindrical domain. A combustible material is one that reacts readily with oxygen, such as carbon or hydrocarbons, and the spontaneous reaction it undergoes is called an exothermic chemical reaction. In this context, heat transfer to the environment is assumed to occur via radiation, involving a two-step combustion process in a one-dimensional reaction. The goal of this study is to theoretically demonstrate how heat is transferred from reactive materials through an exothermic chemical reaction mechanism to the surrounding environment, using a mathematical approach. This method is faster and more cost-effective than experimental procedures. It involves solving the nonlinear ordinary differential equation governing the process by coupling the fourth-order Runge-Kutta (RK45) numerical method with the Shooting Technique. The heat transfer process is influenced by various thermo-physical parameters that affect the system's temperature during combustion. Results show that kinetic variables, such as the Frank-Kamenetskii parameter, also known as the reaction rate, enhance the combustion process, while factors like radiation retard it. An understanding of the heat transfer of reactive materials is crucial in manufacturing industrial equipment to ensure quality and safety.

Keywords: *Combustible material, Cylindrical domain, Radiation, Runge-Kutta, Shooting Technique.*

1. Introduction

Heat transfer in a radiative cylinder of reactive materials is studied in this article. A steady-state combustion process is considered in a two-step low-temperature oxidation reaction. Low-temperature oxidation occurs when a carbon-containing substance reacts spontaneously with the oxygen in the ambient environment, such as in reactive stockpiles like coal, hay, and wood [1, 2]. This phenomenon was also studied in Taghikhani [3] and Logan [4], where an emphasis on automatic combustion of reactive material due to low-temperature oxidation reactions was made. The automatic combustion of reactive materials takes place when their carbon-containing portions react readily with the ambient oxygen trapped within the material's stockpile. Heat released from a low-temperature oxidation combustion process may lead to wildfires, which are detrimental to flora and fauna if the heat trapped within a combustible stockpile continues to accumulate to the extent of self-ignition [5]. Thermal radiation arises due to the difference in the material's surface temperature and its ambient temperature, and it is defined as electromagnetic radiation with a wavelength ranging from 0.1 to 100 microns [6]. The study of thermal radiation has played a major role in modern Physics history [7]. Heat transfer through radiation has numerous industrial applications. In their study of radiative heat transfer in fixed-bed particle solar receivers (PSRs), Dai et al. [8] acknowledged that heat transfer by radiation is necessary for the thermal performance of the fixed-bed PSRs. Radiative heat transfer associated with incident collimated beams is applicable in astrophysics, including the science of the atmosphere [9]. In

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radiative cooling systems, excess heat is dissipated through radiative heat to remote heat sinks [10]. On the other hand, heat transfer applications have been observed in many engineering and industrial platforms. Sahroni [11] outlined the performance of heat transfer in radiator cooling system design, where radiator systems are improved by using coolants and nanofluids to enhance heat transfer coefficients.

Heat transfer modeled in the cylindrical domain has been researched in various approaches. Adeosun et al. [12] investigated a combustible viscoelastic material in a cylindrical stockpile with oxygen consumption and an induced electric field, where a spectral collocation method was used to solve the nonlinear differential equation governing the problem. Their findings were that the augmentation of kinetic parameters, such as the activation energy, reduces the consumption of oxygen, but others, like the reaction rate parameter, increase the consumption of oxygen to enhance the combustion rate. Adesanya et al. [13] studied the reaction kinetics' influence on magneto-convective flow, done in a poro-elastic medium, and taking into consideration nonlinear thermal radiation, including buoyancy effects. One of their contributions is indicating the applications of heat transfer in viscoelastic nanofluids to the fields of pharmacy, biomedicine, and engineering. It was further mentioned that the observation of porous materials' deformation is common in the fields of filtration processes, medicine, energy storage, and geosciences. Moreover, the importance of an additional heat source due to the intense interaction of fluid particles was presented in Neeraja et al. [14]. It was also indicated that the shooting technique was applied to study the distribution of nanoparticles under the influence of Newtonian cooling on the concentration and temperature of the Casson fluid flow in an inclined channel.

The analysis of transient heat in a convective reactive cylinder was studied in Lebelo et al. [15], where nearly similar results as in Adeosun et al. [12] were obtained. Chinyoka and Makinde [16] studied the thermal decomposition and carbon dioxide emission with oxygen depletion in a reactive material modeled in a cylindrical domain. A one-dimensional and one-step combustion process was assumed to arrive at the results. The investigation of an exothermic explosion in a cylindrical pipe was previously studied in Makinde [17], where a series summation technique was applied to the problem solution. In another investigation, Lebelo and Makinde [18] studied the emission of carbon dioxide and the thermal decomposition of reactive material in a cylindrical pipe, where heat transfer to the surrounding environment involved both convection and radiation. In this study, the authors considered a low-temperature oxidation combustion process in a steady-state condition to investigate the transfer of heat in a cylindrical domain, where a two-step reaction mechanism is followed, and heat loss to the environment occurs through radiation. To the authors' knowledge, this study has never been done before. The manuscript layout is as follows: Section 1 is the Introduction, followed by the methodology as the Mathematical Approach in Section 2. The Numerical Approach to the solution of the problem is presented in Section 3, preceding the Results and Discussion fully presented in Section 4. The last part is the Conclusion, presented in Section 5.

2. Mathematical Approach

This study analyzes heat transfer in a stockpile of reactive materials, assuming that a two-step exothermic chemical reaction occurs in a one-dimensional irreversible process.

A two-step reaction mechanism for the combustion of methane in the atmosphere is provided as an example to demonstrate the reaction process [19]:

$$2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O \qquad (1)$$

$$2CO + O_2 + H_2O \rightarrow 2CO_2 + H_2O \qquad (2)$$

The study is modeled in a cylindrical pipe of length x and radial length $\bar{r}$. Throughout the study, constant thermal conductivity is considered. The boundary conditions of the first kind are used to satisfy the radiative heat loss to the ambient, which is described by the Stefan-Boltzmann law. The geometry of the problem is illustrated in Figure 1.

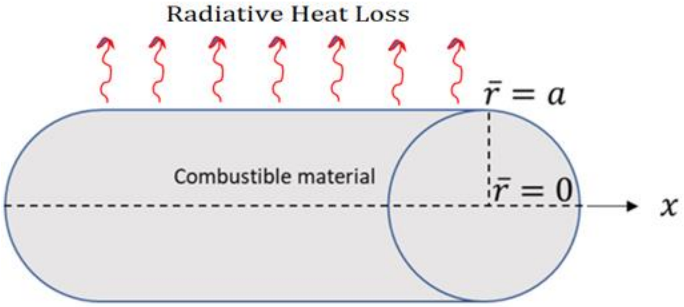

Figure 1.
Geometry of the problem.
Source: Lebelo, et al. [19].

A steady-state energy equation in a one-dimensional domain, following a two-step reaction mechanism and neglecting the reactant consumption, to study radiative heat transfer in a cylindrical domain, is expressed as follows, as presented in Gasior [20] and Francisco and Andrés [21]:

$$\frac{k}{\bar{r}}\frac{d}{d\bar{r}}\left(\bar{r}\frac{dT}{d\bar{r}}\right) + Q_1A_1\left(\frac{KT}{vl}\right)^m e^{-E_1/RT} + Q_2A_2\left(\frac{KT}{vl}\right)^m e^{-E_2/RT} - \mu\sigma(T^4 - T_w^4) = 0. \quad (3)$$

The boundary conditions are given as:

$$\frac{dT}{d\bar{r}}(0) = 0;\ \ T(\bar{r}) = 0. \quad (4)$$

Here T is the cylinder's absolute temperature, T_w is the ambient temperature, μ, σ are the cylinder's emissivity and Stefan-Boltzmann constant, respectively. Q_1, A_1 are, the heat of reaction, the rate constant for the first step, respectively, and Q_2, A_2, represent, respectively, the heat of reaction, the rate constant for the second step. E_1 and E_2 are, respectively, the activation energy for the first step and the second step, m represents the type of chemical kinetics, where $m = -2$ is for the sensitized (light-induced) $m = 0$ is for the Arrhenius and $m = \frac{1}{2}$ is for the bimolecular kinetics, $\bar{r}$ is the cylinder's radial length.

2.1. Dimensionless Parameter Introduction

To solve the governing equations numerically, dimensionless parameters are introduced to convert Equations (3) and (4) into a dimensionless form. A process called nondimensionalization, also known as problem normalization, involves grouping or scaling variables with similar units to create physical properties that are unitless [22]. This technique reduces complexity, including the size of differential equations, to expressions with fewer parameters, from their expressions with dimensions [23]. The nondimensionalization technique is as follows:

$$\left.\begin{array}{c} \theta = \frac{E_1(T-T_W)}{RT_W^2}, \delta = \frac{Q_2 A_2 E_2}{Q_1 A_1 E_1} e^{(E_1-E_2)/RT}, \\ \gamma = \frac{E_2}{E_1}, \lambda = \left(\frac{KT_W}{vl}\right)^m \frac{Q_1\ A_1 E_1\ \ a^2}{kRT_W^2} exp\left(-\frac{E_1}{RT_W}\right), \\ r = \frac{\bar{r}}{a},\ \ \varphi = \frac{RT_W}{E_1},\ \ Ra = \frac{\mu\sigma E_1 a^2 T_W^2}{kR}. \end{array}\right\} \tag{5}$$

The nondimensionalized forms of Equations (3) and (4) are represented as follows:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\theta}{dr}\right) + \lambda(1+\varphi\theta)^m e^{[\theta/(1+\varphi\theta)]} + \lambda\delta(1+\varphi\theta)^m e^{[\gamma\theta/(1+\varphi\theta)]} + \\ -Ra[(\varphi\theta+1)^4 - 1] = 0, \tag{6}$$

Where the boundary conditions are:

$$\frac{d\theta}{dr}(0) = 0, \quad \theta(1) = 0. \tag{7}$$

The nondimensionalized parameters are as follows: Ra is the radiation parameter, λ is the reaction rate parameter, φ is the activation energy, δ is the two-step low-temperature oxidation parameter, γ the activation energy ratio, and r is the radial distance.

3. Numerical Approach to the Solution of the Problem

Application of the coupling of Runge-Kutta-Fehlberg (RKF45) and Shooting technique solved Equations (6) – (7) numerically. The stability algorithm for the RKF45 usually follows these steps [22, 23]:

$$k_1 = \mathrm{h}f(t_i, y_i)$$
$$k_2 = \mathrm{h}f(t_i + \tfrac{1}{4}h, y_i + \tfrac{1}{4}k_1)$$
$$k_3 = \mathrm{h}f(t_i + \tfrac{3}{8}h, y_i + \tfrac{3}{32}k_1 + \tfrac{9}{32}k_2)$$
$$k_4 = \mathrm{h}f(t_i + \tfrac{12}{13}h, y_i + \tfrac{1932}{2197}k_1 - \tfrac{7200}{2197}k_2 + \tfrac{7296}{2197}k_3)$$
$$k_5 = \mathrm{h}f(t_i + h, y_i + \tfrac{439}{216}k_1 - 8k_2 + \tfrac{3680}{513}k_3 - \tfrac{845}{4104}k_4)$$
$$k_6 = \mathrm{h}f(t_i + \tfrac{1}{2}h, y_i - \tfrac{8}{27}k_1 + 2k_2 - \tfrac{3544}{2565}k_3 + \tfrac{1859}{4104}k_4 - \tfrac{11}{40}k_5)$$

The order 4 Runge-Kutta is applied to give the first approximation of the solution, represented thus:

$$y_{i+1} = y_i + \tfrac{25}{216}k_1 + \tfrac{1408}{2565}k_3 + \tfrac{2197}{4104}k_4 - \tfrac{1}{5}k_5. \tag{8}$$

The second approach to the solution uses the order 5 Runge-Kutta method to determine a better approximated value, represented by:

$$z_{i+1} = y_i + \tfrac{16}{135}k_1 + \tfrac{6656}{12825}k_3 + \tfrac{28561}{56430}k_4 - \tfrac{9}{50}k_5 + \tfrac{2}{55}k_6. \tag{9}$$

To compute the numerical approximation of an expression at a particular interval, a set of discrete points of error control tolerance, ϵ, are considered [24], where the error control ϵ is embedded in the following equation:

$$n = 0.840896\left(\frac{\epsilon \mathrm{h}}{|z_{i+1} - y_{i+1}|}\right)^{\frac{1}{4}}.$$

n, and h are the scalar and the step size, respectively, and $n\mathrm{h}$ is the optimal step size. The error estimate $\mathrm{E} = z_{i+1} - y_{i+1}$, is also described by the equation:

$$\mathrm{E} = \tfrac{1}{360}k_1 - \tfrac{128}{4275}k_3 - \tfrac{2197}{75240}k_4 + \tfrac{1}{50}k_5 + \tfrac{2}{55}k_6. \tag{10}$$

Equation (6) was used to demonstrate the convergence of the solution, as illustrated in Figure 2, confirming the stability of the RKF45.

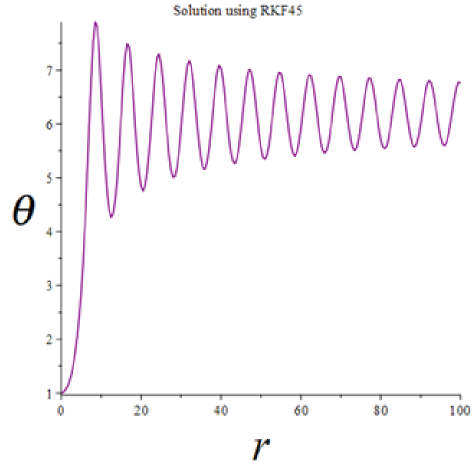

Figure 2.
RKF45 solution from Maple software

Table 1 below shows the increase in the step size from 0.0001 to 1.5000. It is observed that an increase in the step size corresponds to an increase in error **E**, which means that capping the step size very low improves the stability of the RKF45.

Table 1.
RKF45 Convergence.

h	**E**
0.0001	1.7×10^{-13}
0.0010	1.667×10^{-10}
0.0100	1.66666×10^{-7}
0.1000	0.00016658335
1.0000	0.1585290152
1.5000	0.5025050134

The following algorithm converts the second-order differential equation into the first-order one. The following conversions were done: $\theta = g_1,\ \theta' = g_2$. Equations (6) and (7) can be expressed as:

$$\begin{aligned} g'_1 &= g_2 \\ g'_2 &= -g_2 - \lambda(1 + \varphi g_1)^m e^{g_1/(1+\varphi g_1)} - \lambda\delta(1 + \varphi g_1)^m e^{[\gamma g_1/(1+\varphi g_1)]} + \\ &\quad + Ra((g_1 + 1)^4 - 1) \end{aligned} \tag{11}$$

subject to the conditions

$$g_2(0) = 0,\ g_1(1) = 0. \tag{12}$$

4. Results and Discussion

To attain a summarized understanding of radiative heat transfer in this process, the following kinetic parameters were chosen: $\lambda, m, \gamma, \delta, Ra, \varphi$.

4.1. Effects of Selected Parameters on Temperature

Figures 3 to 6 show an increase in the profiles of temperature during the combustion process under the influence of specified parameters. It is noted that, as the magnitudes of the parameters reaction rate, chemical kinetics type, two-step low-temperature oxidation, and activation energy ratio are respectively denoted as λ, m, δ and γ are kept higher, the temperature of the reactive materials within a stockpile shows an increasing pattern. This implies that the low-temperature oxidation process, which causes the combustion of materials, is accelerated, and this may be detrimental to climate change because the combustion process results in accelerated heat transfer to the surrounding environment. For a stockpile of reactive materials, such as hay dumped in an open space, the accumulated heat due to continued temperature elevation may result in self-ignited veld fires that may affect fauna and flora negatively. This is because the more heat accumulated during the combustion process, which cannot escape the system, results in higher levels of temperature that can cause a self-ignition point. A self-ignition point is achieved when the reaction rate parameter's critical values are exceeded, where the reaction rate is described by $\lambda = \left(\frac{KT_W}{vl}\right)^m \frac{Q_1\, A_1 E_1\ a^2}{kRT_W^2} exp\left(-\frac{E_1}{RT_W}\right)$ [25-27]. It is very interesting to note that the increase in the temperature of the system also depends on the type of chemical kinetics; for example, the highest elevation of temperature level is indicated in bimolecular kinetics ($m = 0.5$) as compared to the synthesized kinetics represented by ($m = -2$), illustrated in Figure 4. On the other hand, it is observed that an increase in the magnitudes of Ra and φ show a decrease in the profiles of temperature as illustrated in Figures 7 and 8, respectively. This scenario indicates that the parameters are important to prevent low-temperature oxidation within a reactive stockpile, thereby inhibiting the combustion process that may lead to heat release into the surrounding environment.

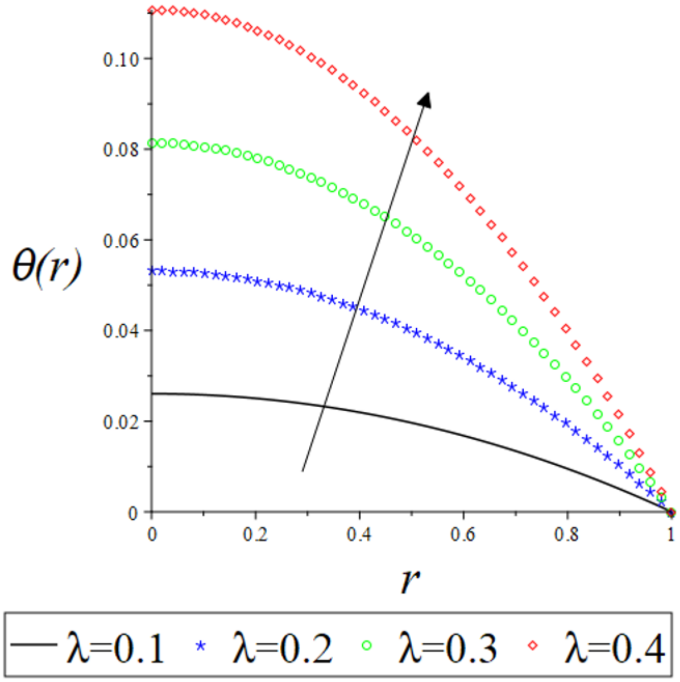

Figure 3.
λ effect on temperature.

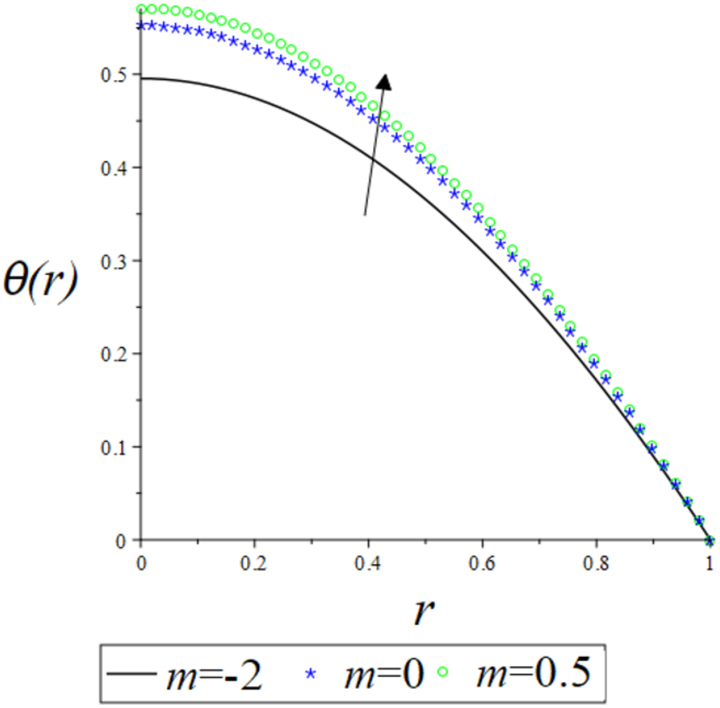

Figure 4.
m effect on temperature.

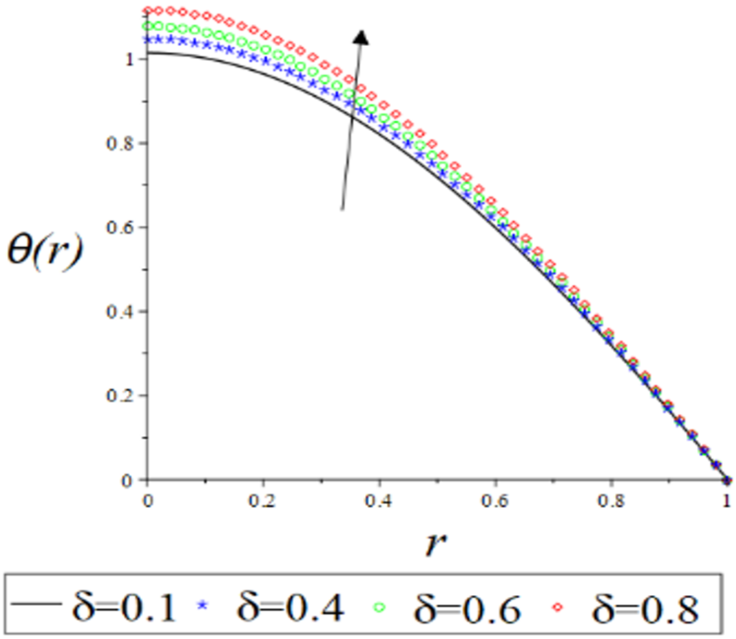

Figure 5.
δ effect on temperature.

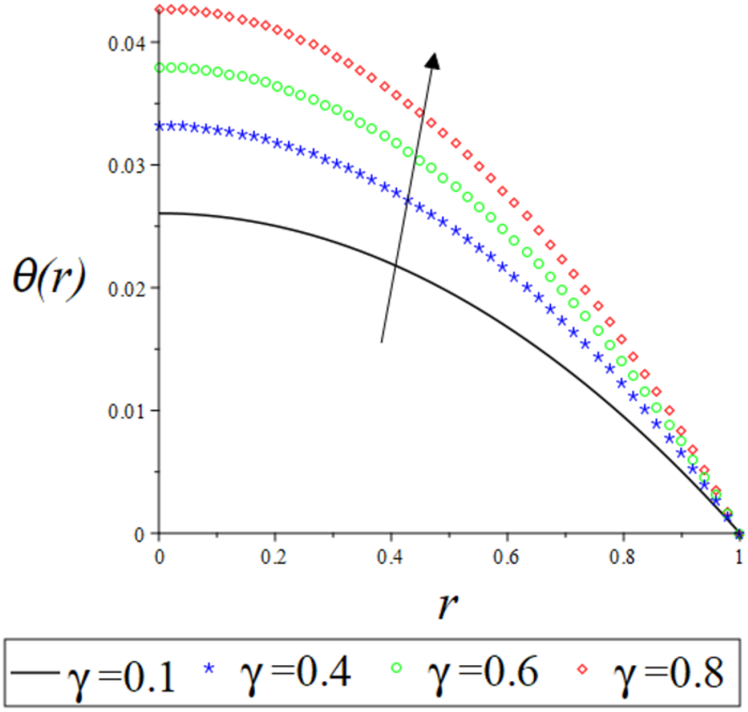

Figure 6.
γ effect on temperature.

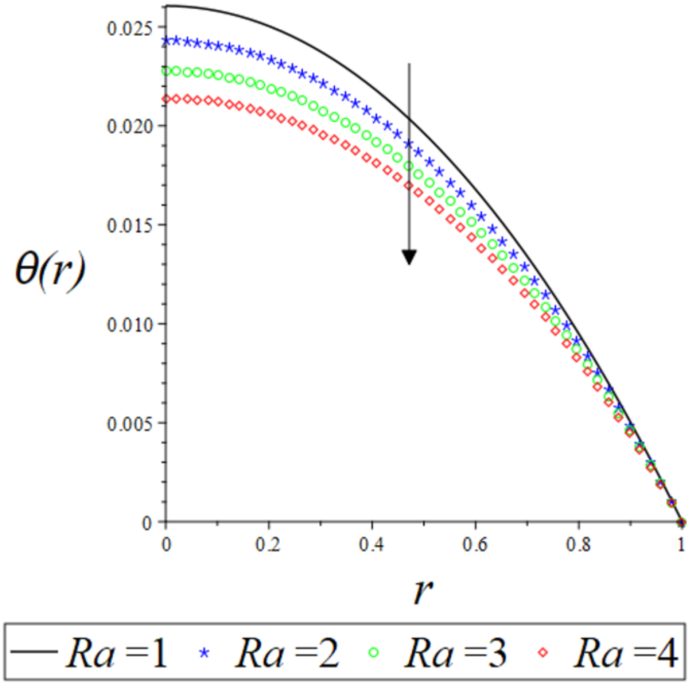

Figure 7.
Ra effect on temperature.

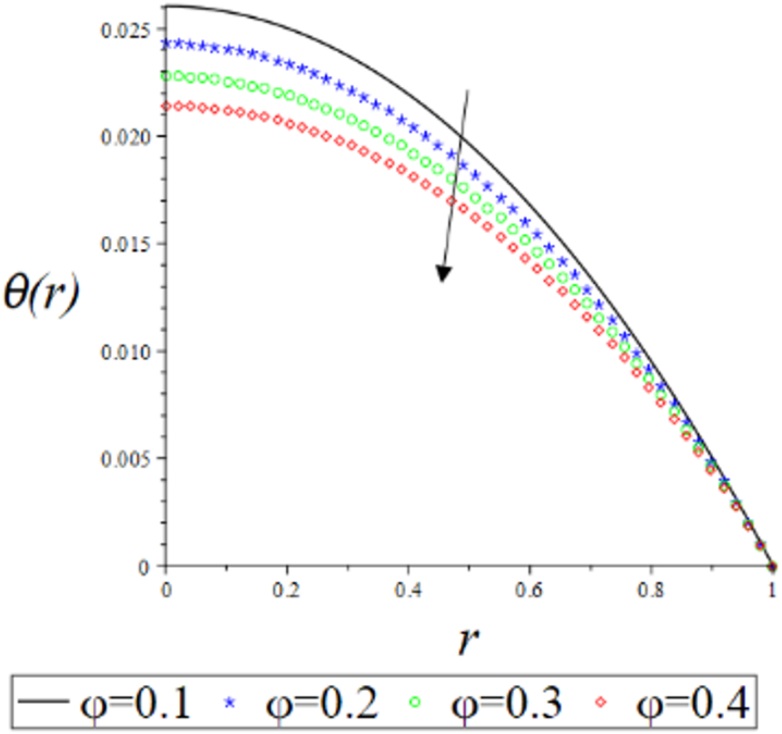

Figure 8.
φ effect on temperature.

4.2. Heat Transfer Rate at the Surface of the Cylinder

The following tables present the heat transfer rates (*Nu*) at different values of the selected parameters. The heat transfer rate exchange at the surface of the reactive material during the combustion process (*Nu*), also called the Nusselt number, is expressed as $-\frac{d\theta}{dr}$. It can be observed from Tables 2 to 5 that increasing the magnitude of each parameter results in a corresponding decrease in the magnitude of *Nu*. This indicates that the rate of heat exchange at the surface of the material diminishes over time under the influence of the parameters listed in the tables. The decreasing *Nu* at the material's surface suggests that more heat is retained within the system, which can accelerate the combustion process. If the heat accumulation becomes excessive, it may lead to system failure or explosion due to elevated temperature profiles. Such explosions during the combustion of reactive material stockpiles in open spaces can cause veld fires, which are harmful to fauna and flora. As previously mentioned, these parameters promote low-temperature oxidation, leading to self-ignition within reactive stockpiles. A different scenario is observed in Tables 6 and 7, where the parameters Ra and φ show that increasing their magnitudes causes an increase in the Nu values, implying that these parameters help reduce the self-ignition process within a stockpile of reactive materials by allowing more heat to escape the system. This is evidenced by a decrease in temperature profiles illustrated in Figures 7 and 8. The more heat is allowed to escape the system, the less the possibility for an explosion to take place, preventing veld fires from occurring in reactive stockpiles neglected in open spaces.

Table 2.
λ on *Nu* (Figure 3).

λ variation	**−Nu values**
0.1	0.05307
0.2	0.10752
0.3	0.16344
0.4	0.22097

Table 3.
m on *Nu* (Figure 4).

m Variation	**−Nu values**
-2	0.93198
0	1.00226
0.5	1.02413

Table 4.
δ on *Nu* (Figure 5).

δ variation	**−Nu values**
0.1	1.19429
0.4	1.20408
0.6	1.21134
0.8	1.21927

Table 5.
γ on *Nu* (Figure 6).

γ variation	**−Nu values**
0.1	0.04678
0.4	0.05957
0.6	0.0681
0.8	0.07664

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Table 6.
Ra on Nu (Figure 7).

Ra variation	$-$Nu values
1	0.05307
2	0.05072
3	0.04863
4	0.04675

Table 7.
φ on Nu (Figure 8).

φ variation	$-$Nu values
0.1	0.05307
0.2	0.05074
0.3	0.04865
0.4	0.04678

5. Conclusion

In this study, the authors investigated heat transfer within a reactive stockpile modeled in a cylindrical domain. Heat transfer to the environment was assumed to be lost through radiation. From this study, it was possible to learn that some embedded parameters, such as the reaction rate, influence the heat transfer process (λ), chemical kinetics (m), the two-step low-temperature oxidation parameter (δ), and the activation energy ratio (γ), enhance the low-temperature oxidation process to cause combustion of reactive materials. It should be noted that the enhancement of low-temperature oxidation on reactive materials is not good for the environment because the heat released during the process of combustion affects climate change in a negative way. On the contrary, some parameters inhibit the low-temperature oxidation from taking place to reduce the combustion of reactive materials by lowering the system's temperature. The parameters in this case were represented by the radiation parameter (Ra) and the activation energy (φ). The inhibition of low-temperature oxidation assists in lowering heat transfer into the environment. This is good for the environment because climate change is not negatively affected. The results in this work agree with the studies done in [17-19]. The work conducted in this article involved a theoretical approach to the study of heat transfer in reactive materials undergoing spontaneous combustion due to low-temperature oxidation processes, using mathematical modeling. This approach is quicker and less expensive compared to experimental methods, and it is also easier for the reader to understand the dynamics of heat transfer during the combustion process. This study may be extended to the combustion of materials modeled in a spherical domain.

Nomenclature:

A_1, A_2	Rate constant $[\mathrm{s}^{-1}]$, (respective steps 1, 2)
Q_1, Q_2	Heat of reaction $[\mathrm{Jkg}^{-1}]$, (respective steps 1, 2)
E_1, E_2	Activation energy $[\mathrm{Jmol}^{-1}]$, (respective steps 1, 2)
h	Heat transfer coefficient $[\mathrm{Js}^{-1}\mathrm{m}^{-1}\mathrm{K}^{-1}]$
k	Thermal conductivity $[\mathrm{Js}^{-1}\mathrm{m}^{-1}\mathrm{K}^{-1}]$
K	Boltzmann constant $[\mathrm{JK}^{-1}]$
l	Planck number $[\mathrm{Js}]$
m	Numerical exponent
R	Universal gas constant $[\mathrm{JK}^{-1}\mathrm{mol}^{-1}]$
Ra	Radiation parameter
T	Absolute temperature of the slab [K]
T_S	Surface temperature of the slab [K]

$\bar{x}$	Cylinder radial distance [m]
x	Dimensionless distance
B, Bi	Biot numbers at $x = 0$ and $x = 1$ respectively
v	Vibration frequency [s^{-1}]

Greek Symbols

γ	Two-step: Dimensionless energy ratio parameters
δ	Two-step: Dimensionless exothermic chemical reaction parameters
φ	Dimensionless activation energy parameter
θ	Dimensionless temperature
μ	Emissivity of the slab
λ	Modified Frank-Kamenetskii parameter
σ	Stefan-Boltzmann constant [W/m^2K^4]

Transparency:

The authors confirm that the manuscript is an honest, accurate, and transparent account of the study; that no vital features of the study have been omitted; and that any discrepancies from the study as planned have been explained. This study followed all ethical practices during writing.

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