# Transient Heat Analysis of a Four-Step Radiative and Convective Kerosene Combustion

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***Abstract:*** *The study investigates heat transfer in a 4-step chemical reaction mechanism of the Kerosene combustion modelled in a cylindrical medium. The reaction mechanism is assumed to be of low-temperature oxidation in nature, and a theoretical mathematical approach is used to investigate the process. A steady-state combustion process is also assumed, and the non-linear energy equation is applied to govern the system. The Runge-Kutta-Fehlberg (RKF45) method coupled with the Shooting Technique is used to solve the governing equation numerically. The thermo-physical parameters embedded within the dimensionless governing equation are used to investigate the heat transfer during the combustion process of Kerosene. The results show that the thermo-physical parameters, such as the reaction rate and kinetic type, accelerate the combustion process, resulting in a higher heat transfer rate to the environment. On the other hand, the parameters such as the activation energy and radiation reduce the tendency for the low-temperature oxidation chemical reaction to take place, which is good for the environment because less heat is lost to the surrounding environment and reduces the effect of climate change.*

**Key-words:** Transient heat, 4-step low-temperature oxidation, convection, radiation, kerosene, cylindrical medium.

## 1. Introduction

The safety and well-being of people working with combustible fluids has led to an increased number of studies on combustion in recent times. This is due to the massive release of hazardous by-products of combustion, heat, and radiation emissions that are linked to the explosive exothermic chemical reactions to which they are exposed. These conditions are often far higher than the normal temperature range and may have far-reaching health effects on the environment and body organs. In this study, attention is focused on the numerical heat investigation of combustible reactive fluid that undergoes a four-step chemical reaction for better performance and efficiency of energy in automobiles' cooling systems, electronic devices, power generation, industrial processing, and in the innovation and improvement of technological solutions, especially in mechanical engineering [1,2]. In chemical engineering, heat exchangers are used to cool hot gas or liquid to a low temperature suitable for storage, where the coolant may be in the form of air or water easily heated in the exchanger [3,4]. This study assumes that heat is lost to the environment by both radiation and convection. Radiative heat loss involves emission of heat waves of wavelength ranging from 0.1 to 100 microns from a hot body to a cold one, where waves can be absorbed $(a)$, reflected $(r)$, or transmitted $(t)$ [5,6], where, $a + r + t = 1$, and for a blackbody, which absorbs all the radiation, $a = 1, r = t = 0$ [1]. Radiation, also characterized by thermal electromagnetic particles distribution as shortwaves and microwaves in a medium, gave birth to thermal radiation therapy, which is applied in the treatment of almost 50% of cancer patients [7,8]. On the other hand, energy transfer between a gas or liquid phase in motion and a solid phase is convective heat transfer, and its application is commonly observed in air-cooled or heat exchangers. Porous media exhibit natural convective heat transfer, hence their numerous applications in engineering, such as cooling of electronic devices and thermal systems [9].

The purpose of this study is to mathematically model the heat transfer for a four-step low-temperature oxidation reaction mechanism of kerosene combustion. Kerosene, also known as Kero, is a flammable liquid and generally non-viscous and clear. Its applications are in households for lighting and cooking where there is no electricity, and as rocket fuel when mixed with oxygen, known as RP1, in engines of jets [10,11]. From the study done in [12], it was found that the addition of oxygen to low-carbonated alcohol and blending it with aviation kerosene (RP-3) produced a fuel whose combustion is shorter than that of diesel, and that the blended product reduced fuel consumption due to its improved thermal efficiency. The four-step combustion of kerosene blended with some hydrocarbons was done by Nadan et al. [13], where the following were assumed: i) minimization of the number of elementary reactions, ii) neglecting of OH radicals, and iii) no additional coefficients to the reaction. The kerosene formula used in [13] is $C_{10}H_{20}$ , and the proposed four-step reaction mechanism for the fuel combustion is:

$$C_{10}H_{20} + 5O_2 \rightarrow 10CO + 10H_2 \qquad \text{STEP 1}$$
$$C_{10}H_{20} + 10H_2O \rightarrow 10CO + 20H_2 \qquad \text{STEP 2}$$
$$H_2 + \frac{1}{2}O_2 \leftrightarrow H_2O \qquad \text{STEP 3}$$
$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \text{STEP 4}$$

It should be noted that each step has its own activation energy ($E_a$) and the four-step activation energy for a low-temperature oxidation illustration is given in the figure below:

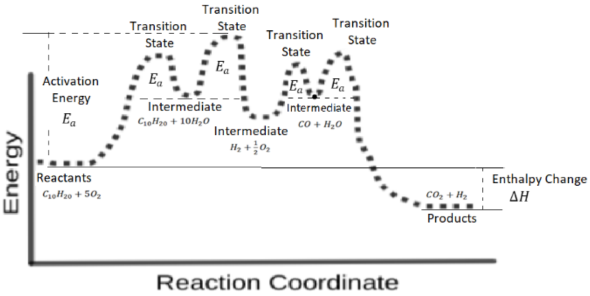

**Figure 1:** 4-step activation energy profile illustrated modification [14]

The study of four-step reaction mechanisms for the combustion of reactive species was explored by many researchers. In 1985, Norbert Peters derived a four-step reaction mechanism for the combustion of methane, known today as the Peters four-step chemistry [15]. Abou-Taouk et al. [16], investigated optimization of a reduced four-step process for a mixture of methane in air, consisting of 10% $CH_4$, 22.5% $CO$ and 67.5% $H_2$. The three and four-step reaction mechanisms with the steps, initiation, branching, and termination, were examined in [17], where it was presented that the three and four-step reaction models are very realistic compared to one-step models and therefore can represent initiating and quenching phenomena in detonations that are unstable. Satisfactory results were also obtained by Boivin et al. [18] when they tested a four-step reaction mechanism including O and OH radicals in a steady state and also investigated the possibility of reducing the four-step mechanism to a three-step one.

The studies done above used experiments to obtain the results. In this study, a theoretical approach using mathematical modelling is used to study the heat transfer during a reactive material combustion. The studies done in [19,20] used a one-step and two-step, respectively, in a cylindrical medium, whereas this study considers a four-step combustion mechanism.

## 2. Mathematical Modelling

This study assumes that a one-dimensional irreversible reaction mechanism with constant thermal conductivity is modelled in a cylindrical domain. The heat loss to the environment is by radiation and convection. The radiative heat loss obeys the Stefan-Boltzmann law expressed as $q = \mu\sigma(T^4 - T_b^4)$, with $\mu$, $(0 < \mu < 1)$, as the emissivity, and $\sigma \approx 5.6703 \times 10^{-8} W/m^2K^4$ as the Boltzmann constant [20], and the convective heat loss follows Newton's law of cooling, showing the rate of heat transfer proportional to the difference between the absolute and ambient temperature, represented by $-\frac{h}{k}[T - T_b]$, with $h$ as the heat transfer coefficient, $k$ as the thermal conductivity of the material, $T$ as the cylinder's absolute temperature, and $T_b$ as the ambient temperature. The geometry of the problem is illustrated in Fig. 2 below:

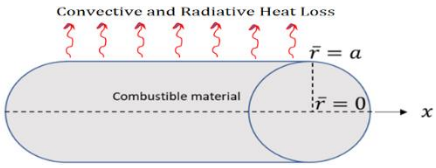

**Figure 2.** Geometry of the problem [20]

A steady state energy equation is used to describe the four-step low-temperature oxidation of the kerosene, neglecting the reactant consumption under study, and it is represented in equation 1.

$$\frac{k}{\bar{r}}\frac{d}{d\bar{r}}\left(\bar{r}\frac{dT}{d\bar{r}}\right)+Q_1A_1C_1\left(\frac{KT}{vl}\right)^m e^{-E_1/RT}+Q_2A_2C_2\left(\frac{KT}{vl}\right)^m e^{-E_2/RT}+Q_3A_3C_3\left(\frac{KT}{vl}\right)^m e^{-E_3/RT}$$
$$+Q_4A_4C_4\left(\frac{KT}{vl}\right)^m e^{-E_4/RT}-\mu\sigma(T^4-T_b^4)-\frac{h}{k}(T-T_b)=0 \tag{1}$$

The boundary conditions are:

$$\frac{dT}{d\bar{r}}(0)=0;\ \ T(a)=0 \tag{2}$$

In this case, $R, l, v, K$ are the universal gas constant, Planck number, vibration frequency, and Boltzmann constant, respectively. $m$ is a chemical reaction kinetics type, with $m=-2, m=0$ and $m=0.5$ respectively representing the sensitized, Arrhenius, and bimolecular kinetics, where $\bar{r}$ is the radial length. Moreover, $Q_1, Q_2, Q_3, Q_4$ represent the heat of reaction for the first step, second step, third step, and fourth step reaction mechanisms, and $A_1, A_2, A_3, A_4$ are the collision frequency constants for the first to fourth step reaction mechanism. $E_1, E_2, E_3$ and $E_3$ are the respective activation energies for the first, second, third, and fourth steps. An equation that is possible to solve numerically is attained by reducing the number of parameters by a dimensionless procedure. This is done as follows:

$$\theta=\frac{E_1(T-T_b)}{RT_b^2},\beta=\frac{Q_2A_2E_2}{Q_1A_1E_1}e^{(E_1-E_2)/RT},\delta=\frac{Q_3A_3E_3}{Q_2A_2E_2}e^{(E_2-E_3)/RT},\epsilon=\frac{Q_4A_4E_4}{Q_3A_3E_3}e^{(E_3-E_4)/RT},B=\frac{ah}{k},$$
$$\gamma=\frac{E_2}{E_1},\alpha=\frac{E_3}{E_2},\omega=\frac{E_4}{E_3},\varphi=\frac{RT_b}{E_1},r=\frac{\bar{r}}{a},\tau=\frac{\mu\sigma E_1a^2T_b^2}{kR},\lambda=\left(\frac{KT_b}{vl}\right)^m\frac{Q_1\,A_1E_1\,a^2}{kRT_b^2}e^{-\left(\frac{E_1}{RT_b}\right)}. \tag{3}$$

In this case, $\theta$ is the dimensionless temperature, $\lambda$ is the reaction rate parameter also called the Frank-Kamenetskii parameter, $\varphi$ is the dimensionless activation energy parameter, $r$ is the dimensionless radial distance, $\gamma, \alpha, \omega$ are the activation energy ratio parameters for the second, third, and fourth steps, $\beta, \delta, \epsilon$ are the low-temperature oxidation parameters for the second, third, and fourth steps, $B$ is the Biot number at $r=0$, and $\tau$ is the dimensionless radiation parameter. Equations (1) – (2) take the following formatting of dimensionless nature:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\theta}{dr}\right)+\lambda(1+\varphi\theta)^m e^{[\theta/(1+\varphi\theta)]}+\lambda\beta(1+\varphi\theta)^m e^{[\gamma\theta/(1+\varphi\theta)]}+\lambda\delta(1+\varphi\theta)^m e^{[\alpha\theta/(1+\varphi\theta)]}+\lambda\epsilon(1+$$
$$\varphi\theta)^m e^{[\omega\theta/(1+\varphi\theta)]}-\tau[(\varphi\theta+1)^4-1]-B\theta=0 \tag{4}$$

The boundary conditions are:

$$\frac{d\theta}{dx}(0)=0,\ \theta(1)=0 \tag{5}$$

## 3. Numerical Solution Algorithm

The coupling of the Runge-Kutta Fehlberg and the Shooting technique was applied to solve numerically the energy equation (4) with its boundary equations (5). The algorithm that was applied to convert equation (4) to first first-order differential equation assumed $\theta=z,\ \theta'=z_1$ and $z'_1=z_2$.

It follows that equations (4)-(5) were expressed as equations (6) and (7).

$$z_2=-z_1-\lambda[(1+\varphi z)^m e^{z/(1+\varphi z)}+\beta(1+\varphi z)^m e^{[\gamma z/(1+\varphi z)]}+$$
$$\delta(1+\varphi z)^m e^{[\alpha z/(1+\varphi z)]}+\epsilon(1+\varphi z)^m e^{[\omega z/(1+\varphi z)]}]+\tau[(\varphi z+1)^4-1]+Bz, \tag{6}$$

with corresponding boundary:

$$z_1(0)=0,\ z(1)=0. \tag{7}$$

Maple software was used to obtain the solutions, which are displayed in the following section.

## 4. Results and Discussion

The selected parameters were used to study the transient heat during a four-step combustion process of kerosene due to low-temperature oxidation reaction: $\lambda = 0.1, \varphi = 0.1, \tau = 1, m = 0.5, \beta = 1, \delta = 1, \epsilon = 1, \gamma = 1, \alpha = 1, \omega = 1, B = 1$.

### 4.1 Steady State Illustration as $t \to \infty$

The following figures illustrate the time-independent solution in 2-Dimensional and 3-Dimensional expressions, demonstrating a steady state process. The steady-state process is demonstrated for $0 < t < 2$ and it is attained when $\theta > 0{,}08$ as $t \to \infty$.

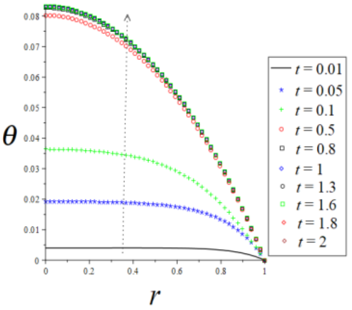

**Figure 3.** 2-D steady state process

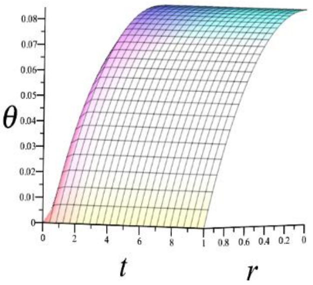

**Figure 4.** 3-D steady state process

**Table 1:** Steady state conditions

| 0<t<2 | θ |
|---|---|
| 0.01 | 0.00402 |
| 0.05 | 0.01927 |
| 0.1 | 0.03694 |
| 0.5 | 0.08021 |
| 0.8 | 0.0828 |
| 1 | 0.0828 |
| 1.3 | 0.0828 |
| 1.6 | 0.0828 |
| 1.8 | 0.0828 |
| 2 | 0.0828 |

Table 1 below shows the steady-state temperature values as $t \to \infty$. It is worth noting that the temperature $(\theta)$ values are no longer increasing beyond the value 0,08021 as $t \to 2$. At this point, the temperature is independent of time.

### 4.2 Discussion of Graphical Results

The graphical solutions illustrated in Figures 5 to 13 demonstrate the heat transfer process as selected parameters mentioned at the beginning of this section are varied. The figures show how the temperature $(\theta)$ profiles behave under the influence of each parameter. Figures 5 to 12 show that when the magnitudes of the parameters $\lambda, m, \beta, \delta, \epsilon, \gamma, \alpha, \omega$ are increased, the temperature profiles increase, indicating that these parameters enhance the exothermic chemical reaction during the kerosene combustion to allow the raising of the temperature of the system. It can be observed from Figure 5 that the rate of reaction parameter $(\lambda)$ is more effective in influencing the material's combustion than other parameters in play. From Table 1 it is observed that the surface heat loss rate $(Nu)$ values -0.17904, -0.37593, -0.59697 and -0.85319 due to $\lambda$'s increase from 0.1 to 0.4 impact on the material's combustion is indicating highest heat loss magnitude at the material's surface as compared to other parameters. Interestingly, Figures 10 to 12 show that the impact of $\beta, \delta, \epsilon$, respectively known as the low-temperature oxidation parameters for the second, third, and fourth steps, are the same on the combustion of the material. This is indicated by $Nu$ values shown as -0.17904, -0.22640, -0.27494, and -0.32475, from Tables 1 and 2 as the parameters' magnitudes are increased from 1 to 4. On the other hand, parameters $\gamma, \alpha, \omega$ being the activation energy ratio parameters for the second, third, and fourth steps, show that their impact on the kerosene combustion is less, as depicted in Figures 7 to 9. The $Nu$ values shown as -0.17904, -0.18109, -0.18334, and -0.18583, from Tables 1 and 2 as the parameters' magnitudes are increased from 1 to 4, also indicate that these parameters' impact on the material's combustion is the same. A different scenario is observed from Figures 13 to 15, where an increase in the magnitudes of the following parameters, dimensionless radiation $(\tau)$, dimensionless activation energy $(\varphi)$, and Biot number $(B)$, show a decline in the temperature profiles. The meaning is that the impact of these parameters on the combustion of kerosene is less, since the exothermic chemical reaction is not accelerated. But the heat transfer to the surrounding environment is enhanced to lower the temperature within the system. It is interesting to note that the impact of $\tau$ and $\varphi$, on the combustion of kerosene is higher as compared to that of $B$. This is evidenced in Figures 13 and 15, including Table 2, with $Nu$ values for $\tau$ and $\varphi$, whose magnitudes, being increased from 1 to 4, are given respectively as -0.17904, -0.17196, -0.16560, -0.15985 and -0.17904, -0.17216, -0.16590, -0.16017. A close look at $Nu$ values indicates that for the $\tau$, the values are larger than those for $\varphi$, meaning that the heat transfer rate from the material's surface is faster under the influence of $\tau$. This confirms that much of the heat is lost due to radiation during the combustion of materials. Figure 14 depicts the impact of $B$ on kerosene combustion, with the $Nu$ values presented in Table 2. The $Nu$ values for $B$ are the largest compared to those for $\tau$ and $\varphi$, meaning that the rate of heat loss at the material's surface in this case is the quickest, and decelerates the exothermic chemical reaction to slow down the kerosene combustion. The temperature profiles are also lower than in Figures 13 and 15, confirming the lesser impact of $B$ on the combustion of kerosene.

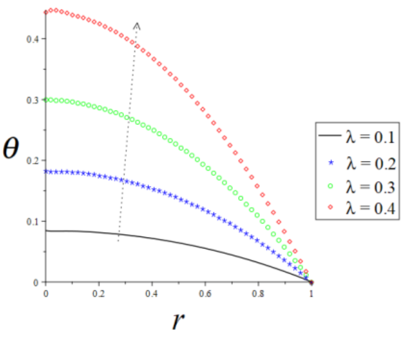

**Figure 5.** $\lambda$ effects

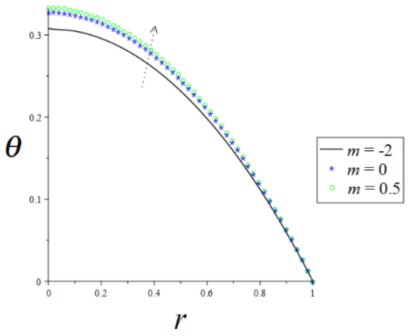

**Figure 6.** $m$ effects

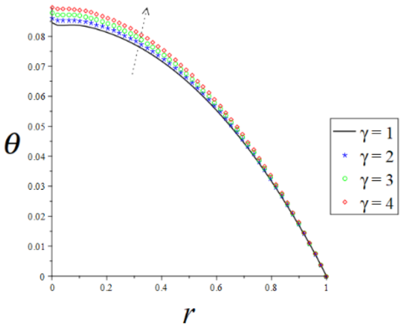

**Figure 7.** ($\gamma$) effects

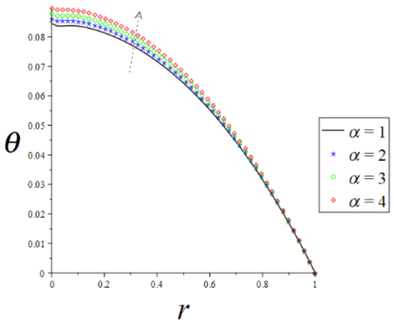

**Figure 8.** $\alpha$ effects

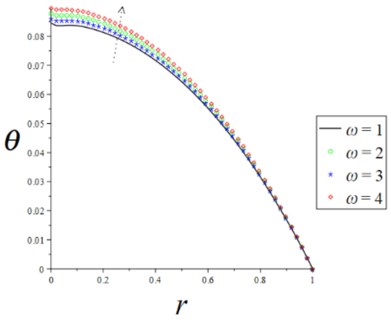

**Figure 9.** $\omega$ effects

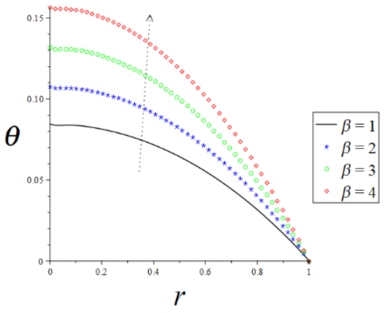

**Figure 10.** $\beta$ effects

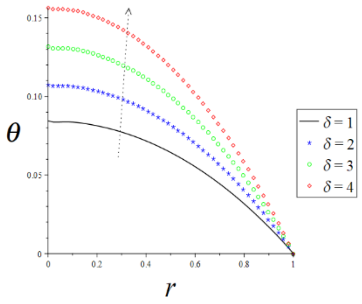

**Figure 11.** $\delta$ effects

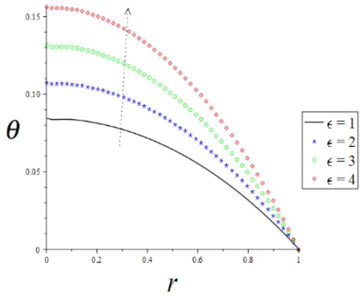

**Figure 12.** $\epsilon$ effects

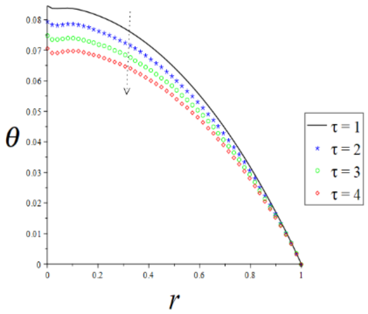

**Figure 13.** ($\tau$) effects

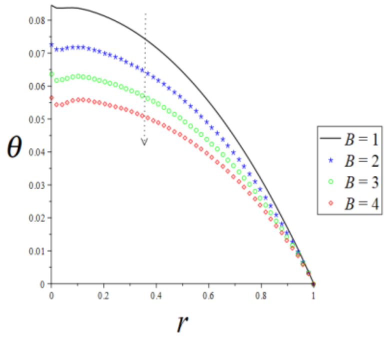

**Figure 14.** $B$ effects

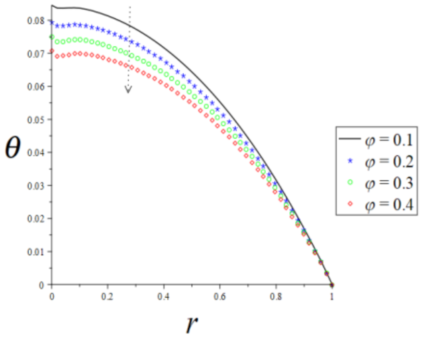

**Figure 15.** $\varphi$ effects

**Table 2:** Effects of $\lambda, m, \gamma, \alpha, \omega, \beta$ on $Nu$ (Figs. 5-10)

| $\lambda$ | $Nu$ | $m$ | $Nu$ | $\gamma$ | $Nu$ | $\alpha$ | $Nu$ | $\omega$ | $Nu$ | $\beta$ | $Nu$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.1 | -0.17904 | -2 | -0.17712 | 1 | -0.17904 | 1 | -0.17904 | 1 | -0.17904 | 1 | -0.17904 |
| 0.2 | -0.37593 | 0 | -0.17865 | 2 | -0.18109 | 2 | -0.18109 | 2 | -0.18109 | 2 | -0.22640 |
| 0.3 | -0.59697 | 0.5 | -0.17904 | 3 | -0.18334 | 3 | -0.18334 | 3 | -0.18334 | 3 | -0.27494 |
| 0.4 | -0.85319 |  |  | 4 | -0.18583 | 4 | -0.18583 | 4 | -0.18583 | 4 | -0.32475 |

**Table 3:** Effects of $\delta, \epsilon, \tau, \varphi$ on $Nu$ (Figs. 11-15)

| $\delta$ | $Nu$ | $\epsilon$ | $Nu$ | $\tau$ | $Nu$ | $B$ | $Nu$ | $\varphi$ | $Nu$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.17904 | 1 | -0.17904 | 1 | -0.17904 | 1 | -0.17904 | 1 | -0.17904 |
| 2 | -0.22640 | 2 | -0.22640 | 2 | -0.17196 | 2 | -0.16275 | 2 | -0.17216 |
| 3 | -0.27494 | 3 | -0.27494 | 3 | -0.16560 | 3 | -0.15001 | 3 | -0.16590 |
| 4 | -0.32475 | 4 | -0.32475 | 4 | -0.15985 | 4 | -0.13973 | 4 | -0.16017 |

## 5. Conclusion

In this study, the heat transfer process was investigated in the combustion of kerosene modeled in a 4-step mechanism process. Different parameters embedded in the governing differential equations were investigated to study their effects on the temperature profiles during the kerosene combustion. Parameters that accelerate the temperature increase during the combustion of the material were found to be the rate of reaction ($\lambda$), chemical reaction kinetics type ($m$), $\beta, \delta, \epsilon$, respectively, known as the low-temperature oxidation for the second, third, and fourth steps, and $\gamma$, $\alpha, \omega$ being the activation energy ratio for the second, third, and fourth steps. Increasing the magnitudes of these parameters indicated an increase in the profiles of the temperature to show that more heat was generated under the effects of the parameters. To reduce spontaneous combustion of reactive materials, it is necessary to have control of these parameters to avoid self-ignition in stockpiles of such materials as coal and hay. The results obtained here agree with those in [21, 22], especially on the impact of $\lambda$ and $m$ on the heat transfer process during reactive materials' combustion. On the other hand, it was found that parameters such as dimensionless radiation ($\tau$), dimensionless activation energy ($\varphi$), and Biot number ($B$), reduce the temperature profiles during the material's combustion to reduce the intensity of the exothermic chemical reaction, which consumes much of the environment's oxygen in the combustion process. The impacts of these parameters are good for retention of oxygen and reduction of heat transfer, which affects the environment in a negative way. The results given by these parameters agree with the work done in [23]. This study can be extended to the investigation of kerosene combustion, where thermal conductivity is dependent on the temperature of the system.

**Conflict of interest:** The authors declare no conflict of interest.

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