Climate Change Due to Exothermic Chemical Reaction of Reactive Materials: A Mathematical Approach

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Abstract

This study highlights physical conditions that contribute to climate change caused by exothermic chemical reactions in reactive materials. The study considers a stockpile of reactive materials such as coal, hay, wood, or dumped rubbish in an open space. An exothermic chemical reaction occurs when the carbon or hydrocarbon of the reactive material reacts spontaneously with the oxygen trapped in the stockpile. The spontaneous combustion raises the temperature of the stockpile. If the accumulated heat does not escape the system, self-ignition may occur, causing the emission of greenhouse gases and heat that contribute to global warming and climate change. The mathematical approach involves using the Navier-Stokes equations to study the heat and mass transfer during the combustion process. The governing non-linear differential equations are solved numerically using the Runge-Kutta Fehlberg (RKF45) method coupled with the Shooting technique. The selection of some parameters, such as the reaction rate and activation energy, helps to bring an understanding of heat and mass transfer. The results obtained show parameters like the reaction rate to facilitate the exothermic chemical reaction, to release more heat and greenhouse gas to the surrounding environment, whereas those like the radiation one retard the reaction mechanism to reduce the release of heat and mass transfer.

Keywords: Climate change, heat and mass transfer, exothermic chemical reaction, reactive material, combustion.

Nomenclature

m	Numerical exponent
T	Absolute temperature of the slab (K)
T_w	Surface temperature of the slab (K)
C	CO_2 concentration ($kgmol^{-1}$)
C_w	CO_2 concentration at the slab surface ($kgmol^{-1}$)
γ	CO_2 diffusivity in the slab
k	Thermal conductivity of the reacting slab ($Js^{-1}m^{-1}K^{-1}$)
$\bar{y}$	Slab rectangular distance (m)
Q	Heat of reaction (Jkg^{-1})
A	Frequency factor (s^{-1})
E	Activation energy ($Jmol^{-1}$)
R	Universal gas constant ($JK^{-1}mol^{-1}$
l	Planck number (Js)
K	Boltzmann constant (JK^{-1})
Ra	Radiation parameter
Nu	Nusselt number
Sh	Sherwood number

Greek Symbols

v Vibration frequency (s^{-1})
ε Emissivity of the slab
σ Stefan-Boltzmann constant ($W/m^2 K^4$)
θ Dimensionless temperature
φ Dimensionless CO_2 concentration
λ Modified Frank-Kamenetskii parameter
μ Dimensionless activation energy parameter
β CO_2 emission rate parameter

Introduction

This article investigates the effect of exothermic chemical reactions on climate change. The exothermic chemical reaction takes place whenever a carbon or hydrocarbon portion of a reactive material reacts readily with the oxygen in the surrounding environment [1]. Research indicates that most of the heating in the mesosphere is due to spontaneous combustion from exothermic chemical reaction [2]. One product of an exothermic chemical reaction combustion process is carbon dioxide (CO_2), and its increase in the atmosphere, corresponding to the increase in the temperature, has been observed for over 200 years [3]. It should be noted further that the living conditions of both fauna and flora are drastically affected by global warming, and that the effect of increased CO_2 in the environment, including human activities, contributes to the overall increase in the mean environmental temperature [4]. A recent study by Ripple et al. [5] reported that a weakening land carbon sink and the drop of land carbon uptake from historical averages have led to a rapid warming pace, resulting in high CO_2 concentration in the atmosphere. The exothermic chemical reaction, taking place in stockpiles of reactive materials such as coal, hay, and dumped rubbish, is one of the sources of greenhouse gas emissions, which led to increased atmospheric temperatures, causing global warming and climate change [6]. More research indicates that emissions of greenhouse gases from human activities cause climate change, resulting in loss of human life and economic damage; hence, the necessity to control and prevent CO_2 emissions into the atmosphere [7,8,9]. The emissions of greenhouse gases contribute to environmental pollution. The study by Kafle et al. [10] gives a mathematical approach to the analysis of the pollutants' concentration in air, taking into account the effects of wind in transporting the pollutants in the atmosphere. Their study also mentioned that the concentration of pollutants depends on four factors, namely, speed of wind, time, emission sources, and diffusion rate. Furthermore, Subbiah [11] investigated the dispersion of pollution by convection under low wind conditions, where the two-wind models together with the Gaussian Plum model were applied in predicting the sulphur dioxide ground-level concentration. Goyal and Kumar [12] discussed a crosswind-integrated concentration concept for developing a general model in analysing the dispersion of pollutants in the boundary layer of the atmosphere. It is important to consider how an exothermic chemical reaction can be manipulated to reduce its effect on greenhouse gas emissions. One of the ways to reduce the effect of exothermic chemical reaction is mentioned in the work by Gabitto and Tsouris [13], who studied how the temperature can be manipulated to increase CO_2 absorption by a solvent in a semi-batch reactor. Their study showed that for an exothermic chemical

reaction in a semi-batch reactor, the drop in temperature of the liquid phase increases the absorption of the CO_2.

The purpose of this study is to investigate the effect of an exothermic chemical reaction on climate change using a mathematical approach to understand the dynamics of combustion that may lead to wildfires. The study by Harris and McDonald [14] developed a simplified two-dimensional wildfire-atmosphere model to capture the main features of wildfire spread. The mathematical approach they applied used two numerical methods, namely, conformal invariance of Laplace's equation and the AAA-least squares method, for solving a singular wildfire problem and for single and multiple spotfire scenarios, respectively. In this study, one-dimensional energy and mass transfer expressions derived from the Navier-Stokes equations were utilized to investigate temperature patterns and CO_2 emissions during the combustion process resulting from the exothermic chemical reaction.

Mathematical approach

One-dimensional energy and mass transfer equations to investigate the temperature patterns and the CO_2 emissions during the combustion process caused by an exothermic chemical reaction in a reactive material modelled in a rectangular slab, with a constant thermal conductivity, are assumed. A time-independent scenario is assumed for both the energy and mass transfer equations to simplify the problem. Figure 1 below represents the geometry of the problem.
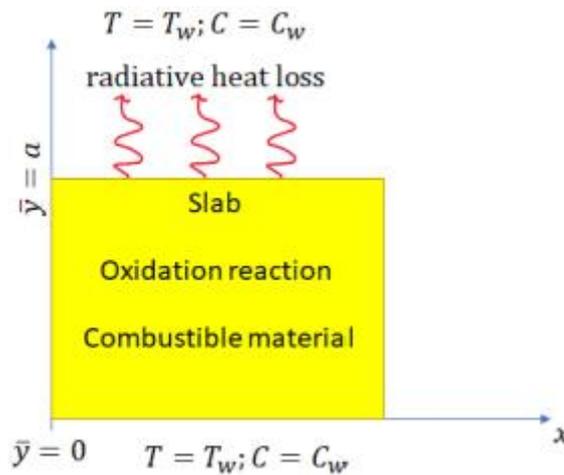

Figure 1. Geometry of the problem

Heat release to the environment is by radiation, following Stefan-Boltzmann's law, expressed as $q = \varepsilon\sigma(T^4 - T_w^4)$, with ε as the slab's emissivity, σ representing Stefan-Boltzmann constant, T the slab's absolute temperature, and T_w the ambient temperature [15]. Following [16,17], the temperature and CO_2 emission equations are respectively expressed thus:

$$k\frac{d^2T}{d\bar{y}^2} + QA\left(\frac{KT}{vl}\right)^m exp\left(\frac{-E}{RT}\right) - \varepsilon\sigma(T^4 - T_w^4) = 0, \tag{1}$$

$$\gamma\frac{d^2C}{d\bar{y}^2} + A\left(\frac{KT}{vl}\right)^m exp\left(-\frac{E}{RT}\right) = 0. \tag{2}$$

The boundary conditions are:

$$\bar{y} = 0, \ T = T_w, \quad C = C_w, \tag{3}$$

$$\bar{y} = a, \ T = T_w, \quad C = C_w. \tag{4}$$

C is the carbon dioxide concentration, and C_w denotes the carbon dioxide concentration at the slab surface with k as the thermal conductivity of the reacting slab. Q represent the heat of reaction, A the frequency factor, E the activation energy, R the universal gas constant, and l is the Planck number. v is the vibration frequency, K is the Boltzmann constant, γ is the slab's CO_2 diffusivity, and $\bar{y}$ is the distance measured vertically. Furthermore, m represents the numerical exponent such that $m \in \{-2,0,0.5\}$, where $m = -2$ represents the numerical exponent for sensitized kinetics, $m = 0$ the Arrhenius kinetics, and $m = 0.5$ the bimolecular kinetics.

The nonlinear equations (1-4) are difficult to solve numerically because they contain dimensional variables with units. It is necessary to use dimensionless variables before solving the equations, and this is done by grouping the physical variables into a reduced number of dimensionless parameters that describe the specified phenomenon [17]. The nondimensionalization is carried out as follows:

$$\theta = \frac{E(T - T_w)}{RT_w^2}, \varphi = \frac{C}{C_w}, \ y = \frac{\bar{y}}{a}, \mu = \frac{RT_w}{E}, Ra = \frac{\varepsilon\sigma E a^2 T_w^2}{kR},$$

$$\lambda = \left(\frac{KT_w}{vl}\right)^m \frac{QAEa^2}{kRT_w^2} exp\left(-\frac{E}{RT_w}\right), \beta = \frac{kRT_w^2}{QE\gamma C_w}. \tag{5}$$

The dimensionless expressions from equations (1-4) are as follows:

$$\frac{d^2\theta}{dy^2} + \lambda(1 + \mu\theta)^m exp\left(\frac{\theta}{1+\mu\theta}\right) - Ra((\mu\theta + 1)^4 - 1) = 0, \tag{6}$$

$$\frac{d^2\varphi}{dy^2} - \lambda\beta(1 + \mu\theta)^m exp\left(\frac{\theta}{1+\mu\theta}\right) = 0. \tag{7}$$

The boundary conditions are:

$$y = 0, \quad \theta = 0, \quad \varphi = 1,$$

$$y = 1, \quad \theta = 0, \quad \varphi = 1. \tag{8}$$

The nondimensional parameters are presented here: λ represents the reaction rate (Frank-Kamenetskii) parameter, μ the activation energy parameter, θ the dimensionless temperature, φ the dimensionless CO_2 concentration, β the CO_2 emission rate parameter, and Ra, the radiation parameter.

Numerical solution

The RKF45 coupled with the Shooting technique was used to solve equations (5-8). The RKF45, for solving equations (5-8), includes the following algorithm [1, 18, 19, 20]:

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf\left(t_i + \frac{1}{4}h, y_i + \frac{1}{4}k_1\right)$$

$$k_3 = hf\left(t_i + \frac{3}{8}h, y_i + \frac{3}{32}k_1 + \frac{9}{32}k_2\right)$$

$$k_4 = \mathbf{h}f\left(t_i + \tfrac{12}{13}h, y_i + \tfrac{1932}{2197}k_1 - \tfrac{7200}{2197}k_2 + \tfrac{7296}{2197}k_3\right)$$

$$k_5 = \mathbf{h}f\left(t_i + h, y_i + \tfrac{439}{216}k_1 - 8k_2 + \tfrac{3680}{513}k_3 - \tfrac{845}{4104}k_4\right)$$

$$k_6 = \mathbf{h}f\left(t_i + \tfrac{1}{2}h, y_i - \tfrac{8}{27}k_1 + 2k_2 - \tfrac{3544}{2565}k_3 + \tfrac{1859}{4104}k_4 - \tfrac{11}{40}k_5\right) \tag{9}$$

To approximate the solution, the Runge-Kutta of order 4 was used, expressed as:

$$y_{i+1} = y_i + \tfrac{25}{216}k_1 + \tfrac{1408}{2565}k_3 + \tfrac{2197}{4104}k_4 - \tfrac{1}{5}k_5. \tag{10}$$

A better solution was obtained with the application of the Runge-Kutta of order 5, given as:

$$z_{i+1} = y_i + \tfrac{16}{135}k_1 + \tfrac{6656}{12825}k_3 + \tfrac{28561}{56430}k_4 - \tfrac{9}{50}k_5 + \tfrac{2}{55}k_6. \tag{11}$$

A set of discrete points at a particular interval, with a tolerance of error control (τ), described by the expression:

$$\tau = \frac{1}{\mathbf{h}}\left(\frac{n}{0.840896}\right)^4 |z_{i+1} - y_{i+1}|,$$

is always used to solve the initial value problem (IVP) [21]. Here, $\mathbf{h}$ represents the step size, n the scalar, $n\mathbf{h}$ the optimal step size, and $z_{i+1} - y_{i+1} = \mathbf{E}$, represents the error estimate. From equations (10) and (11), the error estimate becomes:

$$\mathbf{E} = \tfrac{1}{360}k_1 - \tfrac{128}{4275}k_3 - \tfrac{2197}{75240}k_4 + \tfrac{1}{50}k_5 + \tfrac{2}{55}k_6. \tag{12}$$

The accuracy of the RKF45 for the temperature and CO_2 emissions equations is illustrated in Figures 2 and 3, respectively. For Figure 2, the solution is continuous and bound above and below within the range interval [0, 8.59]. Figure 3 shows that the solution runs smoothly, and it is bounded on the right by 23,029; in other words, the solution cannot be evaluated beyond the specified value.
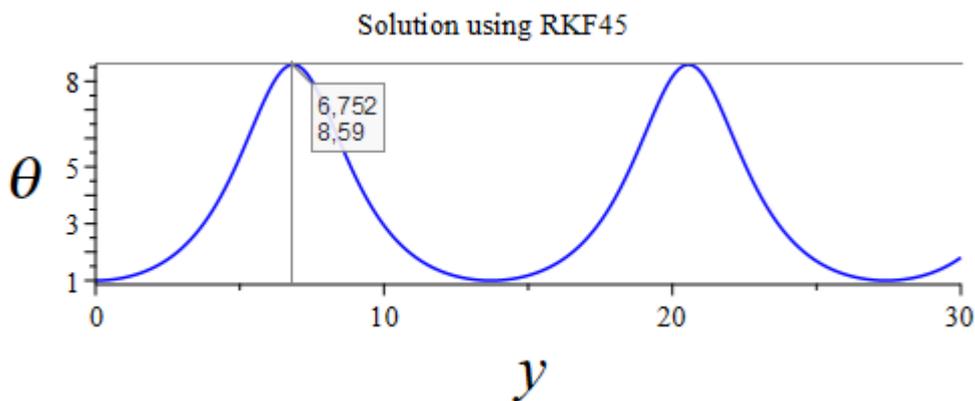

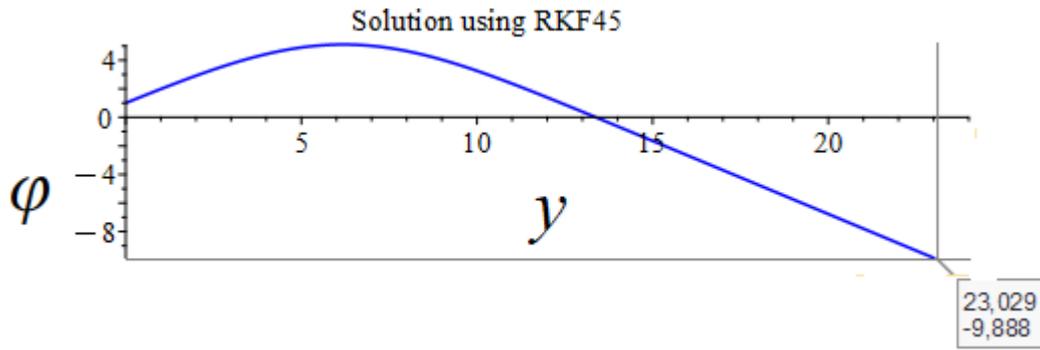Figure 2: Temperature solution

Figure 3: CO_2 concentration solution

The stability of the RKF45 is based on estimating the adaptive error to determine the suitable step size. Table 1 below shows that reducing the step size from 2.000000 to 0.000001 increases the stability of the RKF45, as the error decreases from 1.090702573 to 0.

Table 1: RKF45 Global Convergence

h	E
2.000000	1.090702573
1.500000	0.5025050134
1.000000	0.1585290152
0.100000	0.00016658335
0.010000	1.66666×10^{-7}
0.001000	1.667×10^{-10}
0.000100	1.7×10^{-13}
0.000010	0
0.000001	0

Fig. 4 below demonstrates how the step size increases with the error as illustrated in Table 1.
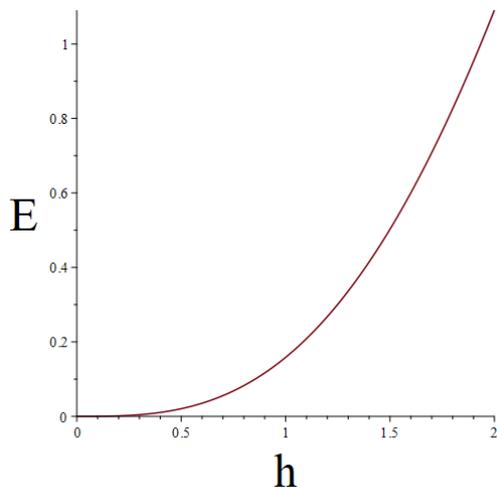

Figure 4: Error increasing with increasing step size

The following algorithm converts the ordinary differential equations of second order to those of the first order: first, letting $\theta = z$, $z' = z_1$ and $z'_1 = z_2$, furthermore, $\varphi = s$, $s' = s_1$ and $s'_1 = s_2$. Therefore, the coupled equations (6) – (8) took the forms:

$$z_2 = -z_1 - \lambda(1 + \varphi z)^m e^{z/(1+\varphi z)} + Ra((\varphi z + 1)^4 - 1),$$
$$s_2 = s_1 + \lambda \epsilon_1 (1 + \varphi z)^m e^{z/(1+\varphi z)}. \tag{13}$$

The boundary conditions are:

$$z_1(0) = 0, \; z(1) = 0, \; s(0) = 1, \; s(1) = 1 \tag{14}$$

The coupled equations (13) – (14) were solved using Maple software to give the results presented and discussed in the following section.

Results and Discussion

This section presents the results and discusses the effects of selected parameters to study the influence of exothermic chemical reaction on combustion of reactive materials, where heat and greenhouse gas are products that are detrimental to the environment, contributing to climate change negatively. The selected parameters are: λ (reaction rate), m (kinetics type), μ (activation energy), β (CO_2 emission rate), and Ra (radiation). For convenience, the parameters were arbitrarily assigned the following standard values: $\lambda = 0.5$, $m = 0.5$, $\mu = 0.1$, $\beta = 0.1$, and $Ra = 1$.

Parameters' effects on Temperature

The effects of parameters λ, m, μ, and Ra, on the temperature of the system are depicted in Figures 5 to 8. From Figures 5 and 6, it is observed that increasing the magnitudes of λ (reaction rate), and m (kinetics type), shows a corresponding increase in the temperature profiles. This means that these parameters support the exothermic chemical reaction to take place, resulting in enhanced heat release and CO_2 emission that affect the environment negatively, contributing to adverse climate change. Table 1 confirms the observations in Figures 5 and 6, where an increase in the magnitudes of λ and m, shows that the rate of heat release at the surface of the material, known as the Nusselt number, expressed as $Nu = -\frac{d\theta}{dy}$ is decreased. The negative sign indicates that heat is released from the system to the surrounding environment. The results indicate that increasing λ from 0.1 to 0.4 shows a decrease in Nu from -0.09131 to -0.40724. The Nu values for an increasing m from -2 to 0.5 are respectively -0.50461, -0.52609, and -0.53204, also showing a decreasing pattern. This decrease confirms an enhanced exothermic chemical reaction, facilitating the combustion process; one of the products in this case is heat, which increases the temperature of the environment, negatively affecting climate change. A decrease in Nu indicates again that much heat, from the combusting material, is diffusing into the surrounding environment. A different scenario is observed in Figures 7 and 8, where an increase in the magnitudes of μ and Ra, indicates a decline in the profiles of the temperature. This means that the parameters decelerate the exothermic chemical reaction during the combustion of reactive materials, and therefore, the heat release to the environment is reduced. This heat release reduction favors a good environment without temperature elevations, contributing very little to climate change. The results indicated in Table 1 show that the rate of heat release (Nu) under the effects of μ and Ra increases with the magnitudes of the

parameters. For Ra the Nu values increase from -0.53204 to -0.37671, and for μ, it is from -0.53204 to -0.37368. This increase indicates a higher heat release rate on the surface of the material, meaning that less exothermic chemical reaction takes place with little heat release as the product, resulting in a decline in the temperature profiles, which is good to avoid explosions during the combustion process. The increase in Nu is significant because less heat from the combusting material diffuses into the atmosphere.
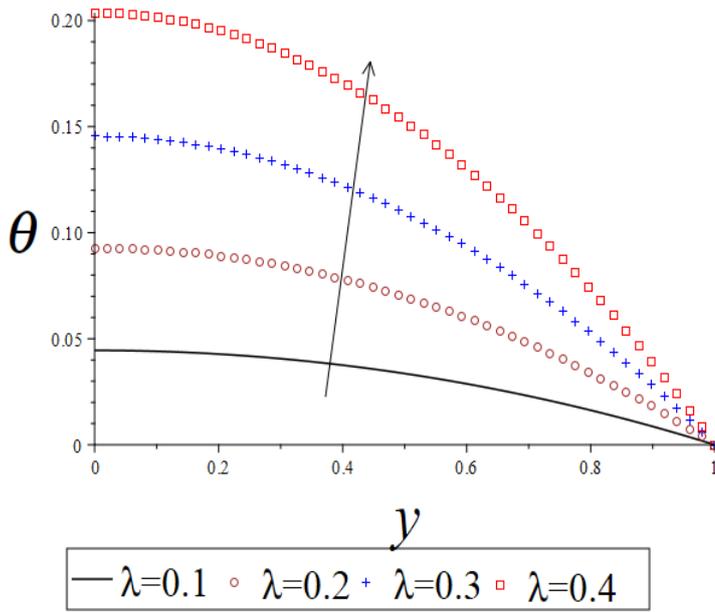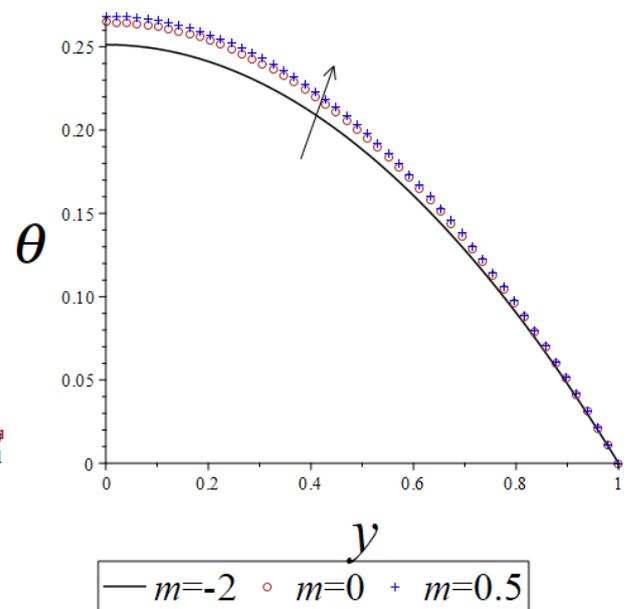

Figure 5: λ effects on temperature

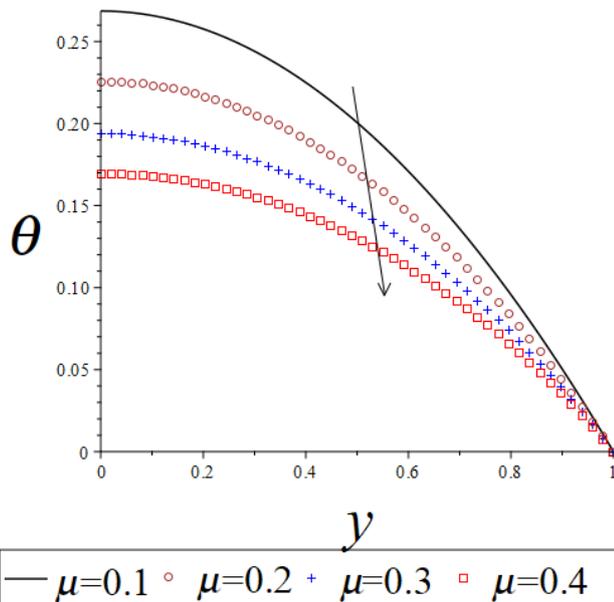Figure 6: m effects on temperature

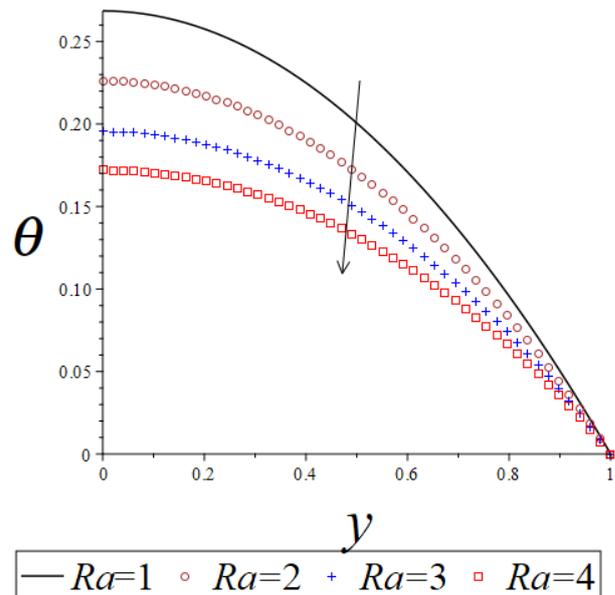

Figure 7: μ effects on temperature

Figure 8: Ra effects on temperature

The following table indicates the effects of the parameters on the rate of heat transfer at the surface of the reactive material, due to the exothermic chemical reaction.

Table 1: Parameters' effects on Nu

λ	m	Ra	μ	Nu
0.1	0.5	1	0.1	-0.09131
0.2	0.5	1	0.1	-0.1888
0.3	0.5	1	0.1	-0.29355
0.4	0.5	1	0.1	-0.40724
0.5	0.5	1	0.1	-0.53204
0.5	0	1	0.1	-0.52609
0.5	-2	1	0.1	-0.50461
0.5	0.5	2	0.1	-0.46425
0.5	0.5	3	0.1	-0.41470
0.5	0.5	4	0.1	-0.37671
0.5	0.5	1	0.2	-0.53537
0.5	0.5	1	0.3	-0.53875
0.5	0.5	1	0.4	-0.54220

Parameters' effects on CO_2

In this section, the effects of parameters on the concentration of CO_2 in an exothermic chemical reaction are discussed. The parameters used in this case are $\lambda, m, \mu, \beta,$ and Ra. From Figures 9-11, it is observed that an increase in the magnitudes of $\lambda, m,$ and β corresponds to an increase in the concentration of CO_2. This means that an exothermic chemical reaction is accelerated to facilitate the combustion process of reactive materials, where heat and CO_2 are the products. The product CO_2 escapes the process to the surrounding atmosphere as a pollutant. This process affects the environment negatively and contributes adversely to climate change. Table 2 indicates the effects these parameters have on the mass transfer rate of CO_2 at the surface of the material, also known as the Sherwood number, expressed as $Sh = -\frac{d\varphi}{dy}$, and negative, confirming the release of the greenhouse gas into the surrounding environment. It is observed that the Sh values for $\lambda, m,$ and β, respectively, decrease from -0.00512 to -0.02236, -0.02778 to -0.02895, and -0.02778 to -0.02784. The decrease in Sh, indicates also that much of the CO_2 diffuses into the surrounding environment, detrimental to climate change. Figures 11 and 12 show that an increase in the magnitudes of μ and Ra, comes with a decrease in the quantity of CO_2 emissions. The decrease is significant in reducing the concentration of greenhouse gas into the atmosphere, which is good for a healthy environment. Furthermore, Table 2 indicates an increase in the Sh as the magnitudes of μ and Ra are increased. It is observed that Sh values for μ, increase from -0.02895 to -0.02784, and those of Ra increase from -0.02895 to -0.02759, meaning that less CO_2 diffuses into the surrounding environment, therefore reducing the intensity of the exothermic chemical reaction, and affecting climate change positively. A good understanding of the characteristics of the parameters embedded within the governing equations is necessary to assist engineers in coming up with preventive measures to avoid veld fires caused by spontaneously ignited fires due to exothermic chemical reactions in stockpiles of reactive materials.
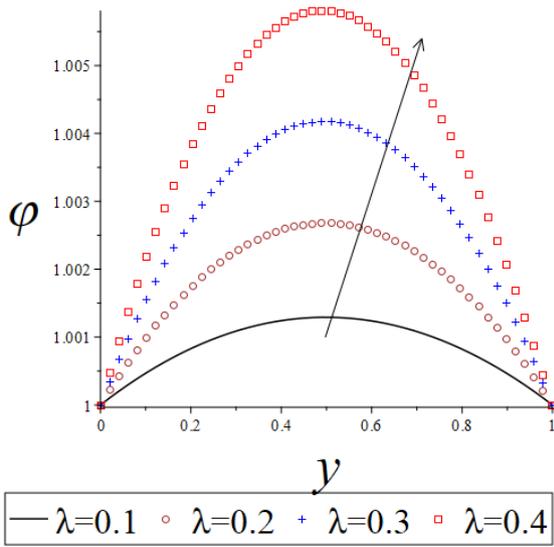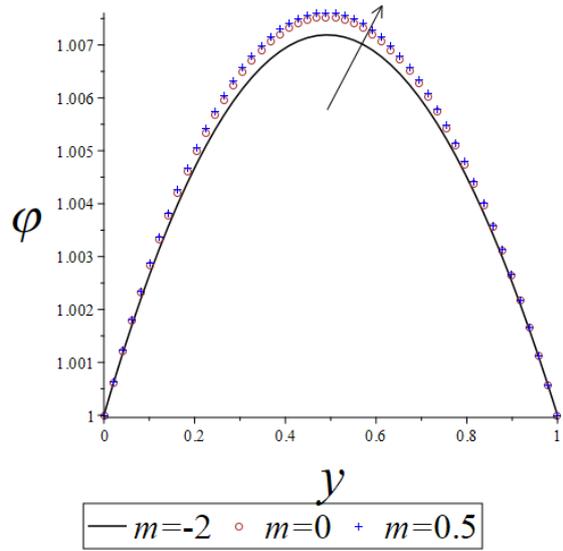
Figure 9: λ on CO_2 concentration

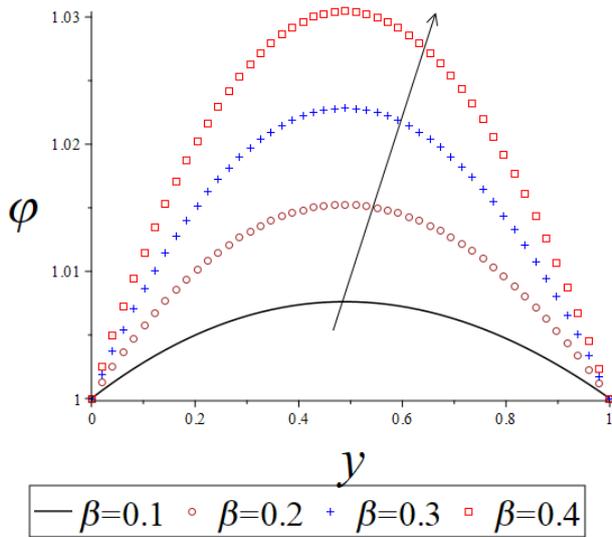Figure 10: m on CO_2 concentration
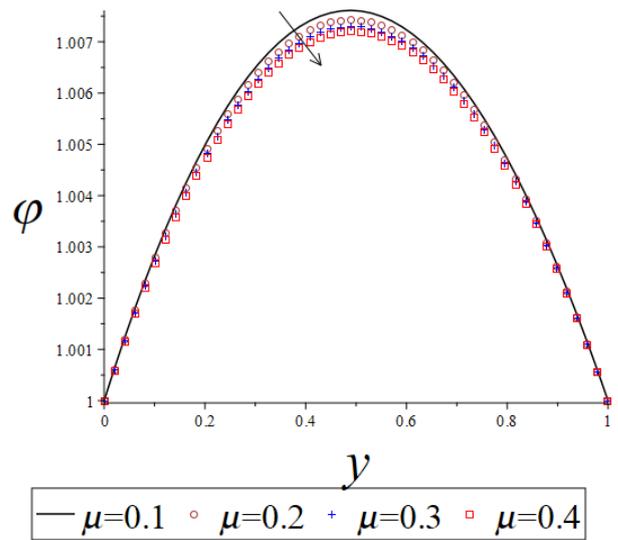

Figure 11: β on CO_2 concentration

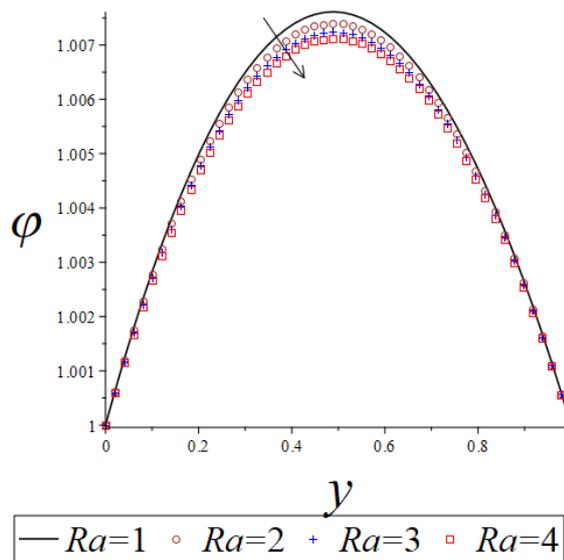Figure 12: μ on CO_2 concentration

Figure 12: Ra on CO_2 concentration

Table 2 below accounts for the influence of selected parameters on the rate of CO_2 transfer at the surface of the reactive material due to the exothermic chemical reaction.

Table 2: Parameters' effects on Sh

λ	m	Ra	μ	β	Sh
0.1	0.5	1	0.1	0.1	-0.00512
0.2	0.5	1	0.1	0.1	-0.01052
0.3	0.5	1	0.1	0.1	-0.01624
0.4	0.5	1	0.1	0.1	-0.02236
0.5	0.5	1	0.1	0.1	-0.02895
0.5	0	1	0.1	0.1	-0.02870
0.5	-2	1	0.1	0.1	-0.02778
0.5	0.5	2	0.1	0.1	-0.02835
0.5	0.5	3	0.1	0.1	-0.02791
0.5	0.5	4	0.1	0.1	-0.02759
0.5	0.5	1	0.2	0.1	-0.05826
0.5	0.5	1	0.3	0.1	-0.08793
0.5	0.5	1	0.4	0.1	-0.11800
0.5	0.5	1	0.1	0.2	-0.02846
0.5	0.5	1	0.1	0.3	-0.02810
0.5	0.5	1	0.1	0.4	-0.02784

Conclusion

The study presented in this work investigated the role of exothermic chemical reactions in climate change. Climate change is primarily driven by elevated temperatures and greenhouse gas emissions. From this study, it was observed that embedded parameters within the energy

and mass transfer equations influence the acceleration or deceleration of the exothermic chemical reaction. Figures 5, 6, 9, and 10 show that parameters such as the reaction rate (λ) and the kinetics type (exponential function, m) accelerate the exothermic chemical reaction, producing more heat and CO_2, which negatively affect climate change. Figure 11 also illustrates how β (CO_2 emission rate parameter) accelerates the exothermic chemical reaction. In contrast, Figures 7, 8, 12, and 13 indicate that there are parameters that decelerate the exothermic chemical reaction, reducing the combustion rate of reactive materials and, in turn, the release of heat and CO_2, which adversely affect climate change. These parameters, μ (activation energy) and Ra (radiation), also embedded in the governing equations, are essential for slowing down heat release and CO_2 emissions. This study can assist engineers in developing products that can alleviate the self-ignition of combustible materials, for example, stockpiles of coal in coal mines. The study can also be extended to reactive materials whose thermal conductivity is temperature dependent.

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