Carbon-dioxide Emission Analysis in a Convective Cylindrical Pipe

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Abstract: - This article analyzed carbon dioxide (CO_2) emission from the combustion of reactive materials modeled in a cylindrical domain. Reactive materials in this case involve carbon-containing substances that react spontaneously with the oxygen of the surrounding environment under the influence of an exothermic chemical reaction. In this analysis, the reactant (oxygen) consumption was neglected. The nonlinear differential equation governing the problem was solved numerically using the Finite Difference Method embedded within the Maple software. It was found that there are kinetic parameters that enhance the emission of CO_2, like the rate of reaction, and others, like the heat loss parameter, retard the CO_2 emission during the exothermic chemical reaction.

Key-Words: - Carbon-dioxide emission, exothermic chemical reaction, convective heat loss, mass transfer, combustible stockpile, cylindrical pipe.

Received: March 24, 2022. Revised: November 17, 2022. Accepted: December 15, 2022. Published: December 31, 2022.

1 Introduction

Carbon dioxide (CO_2) emission has drawn the attention of many researchers because of its devastating impact on the environment. Continued CO_2 emission in the atmosphere is considered one of the challenges in the 21st century that threatens human safety and health because it brings degradation of the environment and is therefore a natural disaster, [1,2]. The emission of CO_2 is also considered to be one of the fundamental factors that breed climate change and is therefore one of the world's problems with the environment, [3,4]. Rehman et al. mentioned that it is necessary to limit CO_2 emissions to tackle climate change to sustain worldwide economic growth, [4]. Fernández-Amador et al. claim CO_2 to be the main greenhouse gas that is present in the atmosphere with longer atmospheric life, though its global warming potential per mole is lower compared to other greenhouse gases, [5]. According to the study done by Distefano et al., climate change led to water scarcity, which also caused the shrinking of economic activities in the countries under the Organization for Economic Cooperation and Development (OECD), [6]. Further studies by Kahia et al., Marques et al., and Mikayilov et al. have shown that economic growth is to some extent inhibited and undermined by climate change to delay social development, [7,8,9]. Though CO_2 emissions are detrimental to the environment, studies show that economic growth goes hand in hand with CO_2 emissions, [4]. This is the reason China, believed to be one of the CO_2 emissions accelerators due to its economic growth excellency, is determined to peak CO_2 emissions by 2030, and before 2060, it is determined to achieve the neutrality of carbon, [4]. Since economic growth is accompanied by CO_2 emissions, different activities of the economy such as trade and urbanization, energy consumption, industrial structure, fossil, and cleaner fuels consumption structure, technological advancement, and foreign investment enhance the emissions of greenhouse gas, [10,11,12,13].

Although CO_2 is a large contributor to greenhouse gases, it is also usable in many instances, for example, it is turned into a protein-rich powder for animal feed, [14]. Other applications of CO_2 are found in dry blasters, fire extinguishers, soft drinks, and as end products of fertilizers, fuels, and materials, [15]. Lately, the study by Palm, Nilsson, and Åhman showed that CO_2 is also applicable in drop-in plastics, [16], CO_2 is also used for lowering climate change in concrete mixtures, [17], and it is also used for enhancing oil recovery, [18].

This study focuses on CO_2 emission analysis in a stockpile of reactive materials modeled in a cylindrical pipe. This study aims to investigate the factors (kinetic parameters) that enhance or reduce the emission of CO_2 during a spontaneous combustion process due to an exothermic chemical reaction of reactive materials in a stockpile. The CO_2 emission analysis in a reactive stockpile modeled in a rectangular slap was studied by Lebelo and Makinde, [19]. Their study considered a steady-state combustion process with heat loss to the ambient by radiation. In, [20], the study was considered in a cylindrical domain with heat loss to the environment by both convection and radiation. The study in a spherical domain was conducted in, [21], where the heat loss to the surrounding environment was due to convection. The study considered simultaneous CO_2 emission, O_2 consumption, and transient heat stability during the spontaneous combustion of reactive materials. The studies done above considered a combustion process in a one-step scenario, in this study, a two-step combustion process analogous to the one taking place in fuel combustion in an automobile exhaust system.

2 Problem Formulation

A one-dimensional energy and mass transfer partial differential equations with constant thermal conductivity are used to model the problem. The reactant concentration is neglected. The problem is modeled in a long cylindrical pipe illustrated in Fig. 1 below.

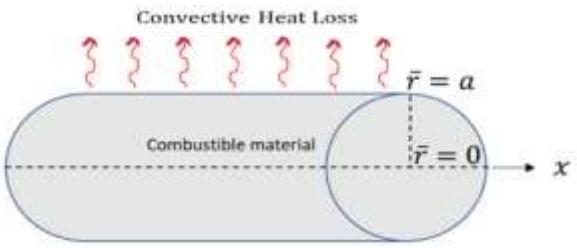

Fig. 1: Geometry of the Problem

Coupled equations describing the heat and mass transfer are given as follows:

$$pc_p\frac{\partial T}{\partial \bar{t}} = k\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{r}\frac{\partial T}{\partial r}\right) + Q_1A_1\left(\frac{KT}{vl}\right)^m e^{-E_1/RT} + Q_2A_2\left(\frac{KT}{vl}\right)^m e^{-E_2/RT} - x(T-T_b). \quad (1)$$

$$\frac{\partial M}{\partial \bar{t}} = P\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{r}\frac{\partial M}{\partial r}\right) + A_1\left(\frac{KT}{vl}\right)^m e^{-E_1/RT} + A_2\left(\frac{KT}{vl}\right)^m e^{-E_2/RT}. \quad (2)$$

The initial and boundary conditions for equations (1) and (2) are respectively expressed as:

$$T(\bar{r},0) = T_0, M(\bar{r},0) = 0, \quad (3)$$

and

$$\frac{\partial T}{\partial \bar{r}}(0,\bar{t}) = 0;\ \frac{\partial T}{\partial \bar{r}}(a,\bar{t}) = -\frac{h}{k}[T(a,\bar{t}) - T_b];$$
$$\frac{\partial M}{\partial \bar{r}}(0,\bar{t}) = 0;\ \frac{\partial C}{\partial \bar{r}}(a,\bar{t}) = -\frac{g}{f}[M(a,\bar{t}) - M_b] \quad (4)$$

Convective heat loss to the surrounding environment follows Newton's law of cooling, expressed as $-\frac{h}{k}[T-T_b]$, where h is the heat transfer coefficient and k is the thermal conductivity, T_b is the ambient temperature, T_0 is the initial temperature, and T is the cylinder's thermodynamic temperature. The mass transfer at the cylinder's surface is given by $-\frac{g}{f}[M-M_b]$, where g is the CO_2 transfer coefficient and f is the diffusivity of CO_2 in the cylinder. M is the CO_2 emission concentration, M_b is the concentration of CO_2 in the environment, p, and c_p are the density and the specific heat at constant pressure. Q_1 and A_1 are, respectively, the heat of the reaction, and the Arrhenius constant, for the first step of the reaction, and Q_2 and A_2 represent the heat of the reaction and the Arrhenius constant, respectively, for the second step. In addition, K is the Boltzmann's constant, v is the vibration frequency, l is Planck's number, E_1 and E_2 are, respectively, the activation energy for the first step and the second step, R is the universal gas number, 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 and lastly, $x = h.\boldsymbol{s}$ is the heat loss parameter, where $\boldsymbol{s}$ is the inner surface.

The introduction of dimensionless quantities on equations (1) – (4) is done as follows:

$$\theta = \frac{E_1(T-T_b)}{RT_b^2}, \theta_0 = \frac{E_1(T_0-T_b)}{RT_b^2}, r = \frac{\bar{r}}{a}, \varepsilon = \frac{RT_b}{E_1},$$
$$\gamma = \frac{E_2}{E_1}, t = \frac{k\bar{t}}{pc_pa^2}, \mu = \frac{Q_2A_2E_2}{Q_1A_1E_1}e^{(E_1-E_2)/RT}, \epsilon = \frac{a^2x}{k}$$
$$\lambda = \left(\frac{KT_b}{vl}\right)^m\frac{Q_1A_1E_1a^2}{kRT_b^2}e^{-E_1/RT},\ \alpha = \frac{ah}{k}, \sigma = \frac{ag}{f}$$
$$\omega = \frac{A_2}{A_1}e^{(E_1-E_2)/RT}, \varphi = \frac{M}{M_b}, \beta = \frac{kRT_b^2}{QE_1P}. \quad (5)$$

Equations (1) – (4) then become

$$\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial r^2} + \frac{1}{r}\frac{\partial\theta}{\partial r} + \lambda(1+\varepsilon\theta)^m e^{[\theta/(1+\varepsilon\theta)]} + \lambda\mu(1+\varepsilon\theta)^m e^{[\gamma\theta/(1+\varepsilon\theta)]} - \epsilon\theta \quad (6)$$

$$\frac{\partial\varphi}{\partial t} = \frac{\partial^2\varphi}{\partial r^2} + \frac{1}{r}\frac{\partial\varphi}{\partial r} + \lambda\beta(1+\varepsilon\theta)^m e^{\theta/(1+\varepsilon\theta)} + \lambda\omega(1+\varepsilon\theta)^m e^{[\gamma\theta/(1+\varepsilon\theta)]} \quad (7)$$

The corresponding initial and boundary conditions are respectively expressed as follows:

$$\theta(r,0) = 0,\ \varphi(r,0) = 1, \text{ and}$$

$$\frac{\partial\theta}{\partial r}(0,t) = \frac{\partial\varphi}{\partial r}(0,t) = 0,$$
$$\frac{\partial\theta}{\partial r}(1,t) = -\alpha[\theta(1,t) - \theta_0],$$
$$\frac{\partial\varphi}{\partial r}(1,t) = -\sigma\,[\varphi(1,t) - 1]. \quad (8)$$

The dimensionless parameters are described as follows:
θ and θ_0 are the dimensionless temperature and dimensionless initial temperature respectively, λ is the Frank-Kamenetskii parameter also called the reaction rate parameter, $\varepsilon, r, \gamma, \mu$ are, respectively parameters for, the dimensionless activation energy, the dimensionless radial distance, the activation energy ratio, and the two-step low-temperature oxidation parameter. $\alpha, \sigma, \beta, \omega, t$ are, respectively, the Biot and CO_2 Biot numbers, CO_2 emission rate parameter, CO_2 two-step emission rate parameter, and dimensionless time. ϵ is the dimensionless heat loss parameter

2.1 Steady-state combustion formulation

As time $t \to \infty$, the combustion process attains a steady state situation, where the energy and mass transfer equations are temperature independent. The expressions for the energy and mass transfer equations, and their boundary conditions are respectively expressed as follows:

$$0 = \frac{\partial^2\theta}{\partial r^2} + \frac{1}{r}\frac{\partial\theta}{\partial r} + \lambda(1+\varepsilon\theta)^m\left\{e^{[\theta/(1+\varepsilon\theta)]} + \mu e^{[\gamma\theta/(1+\varepsilon\theta)]}\right\} - \epsilon\theta \quad (9)$$

$$0 = \frac{\partial^2 \varphi}{\partial r^2} + \frac{1}{r}\frac{\partial \varphi}{\partial r} + \lambda\beta(1+\varepsilon\theta)^m e^{\theta/(1+\varepsilon\theta)} + \\ + \lambda\omega(1+\varepsilon\theta)^m e^{[\mu\theta/(1+\varepsilon\theta)]} \quad (10)$$

The boundary conditions are:

$$\frac{\partial \theta}{\partial r}(0) = \frac{\partial \varphi}{\partial r}(0) = 0, \\ \frac{\partial \theta}{\partial r}(1) = -\alpha[\theta(1) - \theta_0], \\ \frac{\partial \varphi}{\partial r}(1) = -\sigma\,[\varphi(1) - 1]. \quad (11)$$

The Runge-Kutta (RK-4) coupled with Shooting technique is applied to numerically solve the steady state problem.

3 Problem Solution

The problem to be solved in this case concentrates on equation (7) and its corresponding boundary and initial conditions. The focus is on CO_2 analysis in a spontaneous combustible process of reactive materials. Following, [22], equation (7) was solved numerically using the Finite Difference Method (FDM) due to the nonlinearity of the equation. The following FDM expression describes the solution algorithm.

$$\frac{\varphi_i^{j+1} - \varphi_i^j}{\Delta t} = \tau\left(\frac{\varphi_{i+1}^{j+1} - 2\varphi_i^{j+1} + \varphi_{i-1}^{j+1}}{(\Delta r)^2}\right) + \\ +(1-\tau)\left(\frac{\varphi_{i+1}^{j} - 2\Phi_i^{j} + \varphi_{i-1}^{j}}{(\Delta r)^2}\right) + \\ +\lambda\beta(1+\varepsilon\theta_i^j)^m {\varphi_i^j}^n e^{\left[\theta_i^j/(1+\varepsilon\theta_i^j)\right]} + \\ +\lambda\omega(1+\varepsilon\theta_i^j)^m {\varphi_i^j}^n e^{\left[\mu\theta_i^j/(1+\varepsilon\theta_i^j)\right]} \quad (12)$$

The temperature at current time step is expressed by j, and $j+1$ describes the new temperature. The space position in the r direction is denoted by i. The $(j+\tau)$ describes the intermediate time level, where $\tau \in [0;1]$. To allow larger time steps that can accommodate any value, we let $\tau = 1$, to determine the implicit terms.

The rearrangement of equation (12) after multiplying through by Δt and writing $c = \frac{\Delta t}{\Delta r^2}$, gave the following equation:

$$-\tau c\varphi_{i+1}^{j+1} + (1+2\tau c)\varphi_i^{j+1} - \tau c\varphi_{i-1}^{j+1} \\ = c(1-\tau)\varphi_{i+1}^j + [1-2c(1-\tau)]\varphi_i^j + c(1-\tau)\varphi_{i-1}^j + \\ +\lambda\beta\Delta t\,(1+\varepsilon\theta_i^j)^m {\varphi_i^j}^n e^{\left[\theta_i^j/(1+\varepsilon\theta_i^j)\right]} + \\ -\lambda\omega\Delta t\,(1+\varepsilon\theta_i^j)^m {\varphi_i^j}^n e^{\left[\mu\theta_i^j/(1+\varepsilon\theta_i^j)\right]} \quad (13)$$

The initial and boundary conditions are as follows:

$$\varphi_i^j = 1;\ \varphi_{i+1}^j = \varphi_{i-1}^j\ (r=0); \\ \frac{1}{\Delta r}(\varphi_{i+1}^j - \varphi_{i-1}^j) = -\sigma[\varphi_i^j - 1]\ (r=1) \quad (14)$$

The FDM is embedded withing Maple software, this method was used to solve equations (13) to (14) using the software.

The Shooting- Runge–Kutta Method, also embedded within Maple software, is applied to solve the steady-state equation (10), the algorithm is as follows:

Let $\theta = x_1,\ \theta' = x_2,\ \varphi = x_3,\ \varphi' = x_4$

Then, equation (10) is transformed into a first order differential equation as follows:

$$x'_3 = x_4 \\ x'_4 = -\frac{1}{r}x_3 + \lambda\beta(1+\varepsilon x_1)^m e^{x_1/(1+\varepsilon x_1)} + \\ -\lambda\omega(1+\varepsilon x_1)^m e^{[\mu x_1/(1+\varepsilon x_1)]}. \quad (15)$$

The corresponding boundary conditions are:

$$x_4(0) = 0,\ x_4(1) = -\sigma\,[x_3(1) - 1] \quad (16)$$

4 Results and Discussion

The results obtained in the CO_2 analysis in a combustible stockpile modelled in a cylindrical domain, are presented, and discussed in this section. The steady-state combustion process is looked at first, then followed by the unsteady-state condition. In both processes, the following dimensionless parameters' settings were applied:

$$\lambda = 0.1, m = 0.5, \varepsilon = 0.1, \gamma = 0.1, \mu = 0.1, \\ \theta_0 = 0.1 \\ \alpha = 1, \sigma = 1, \beta = 1, \omega = 1, \epsilon = 1$$

4.1 Steady-state combustion process

The following Figs. 2 and 3 depict the steady-state attainment as $t \to \infty$.

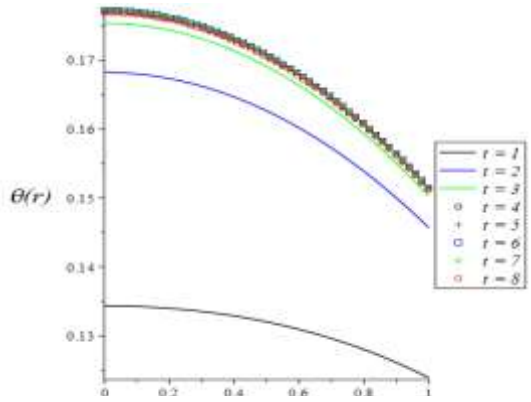

Fig. 2: 2-D steady-state illustration

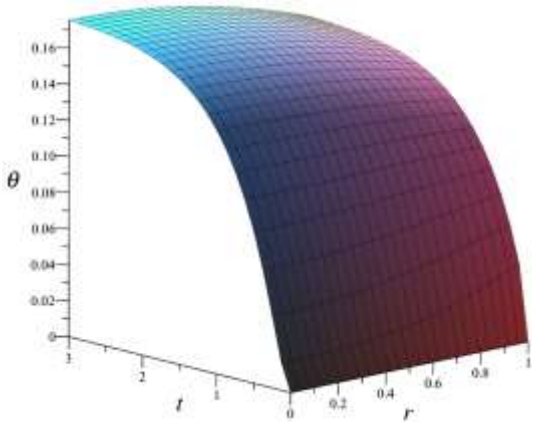

Fig. 3: 3-D steady-state illustration

It is clearly observable that the steady-state condition is attained as time t increases from zero to infinity. Table 1 indicates that the temperature values reach a constant number (0.15123) over time $t = 4 \rightarrow \infty$. This shows that the CO_2 constantly keeps on being emitted when the combustion process continues even if the time component is ignored. Fig. 2 illustrates too that the CO_2 is highly concentrated at the center of the stockpile and declines towards the surface of the combusting material, due to its high rate of emission to the surrounding environment.

Table 1: Steady-state temperatures as $t \rightarrow \infty$ at $r = 1$

Time t	**Temperature** θ
$t = 1$	$\theta = 0.12390$
$t = 2$	$\theta = 0.14562$
$t = 3$	$\theta = 0.15020$
$t = 4$	$\theta = 0.15123$
$t = 5$	$\theta = 0.15123$
$t = 6$	$\theta = 0.15123$
$t = 7$	$\theta = 0.15123$
$t = 8$	$\theta = 0.15123$

4.2 Unsteady-state combustion process

Each kinetic parameter mentioned above was varied to study the process of CO_2 emission under its influence. The effects of the following parameters on CO_2 emission are depicted in Figs. 4-14.

Figs. 4-11 illustrate the effects of $\lambda, \gamma, \varepsilon, \beta, \omega, \mu, m,$ and θ_0. It is observed that an increase in the parameters mentioned brings a corresponding increase in the emission of CO_2. The CO_2 emission corresponds to the temperature levels increments, as heat is released to the environment, during the exothermic chemical reaction. Both heat release and CO_2 emission are detrimental to the environment. What is more interesting is to observe that the CO_2 emission is least in sensitized kinetics ($m = -2$) as compared to bimolecular kinetics ($m = 0.5$), as indicated by Fig. 10. Figs. 4 and 7, show that the reaction rate and the CO_2 emission rate parameters contribute much to the emission of the greenhouse gas. From Figs. 5, 8 and 11, we observe that the two-step low-temperature oxidation parameter, CO_2 two-step emission rate parameter, and dimensionless initial temperature, respectively, have almost the same effect on the CO_2 emission. It is observed also from Figs. 6 and 9 that the activation energy, and the activation energy ratio also show the same effect on the CO_2 emission. Tables 2-9 confirm the CO_2 emission increment as the magnitudes of the mentioned parameters are increased. The Sherwood number $\left(Sh = -\frac{d\varphi}{dr}\right)$ which is the CO_2 rate transfer at the cylinder's wall to the surrounding environment, also shows that the CO_2 emission rate increases with increasing values of the parameters under the study. For example, Table 2 shows that as λ is increased from 0.1 to 0.5, the CO_2 concentration increases from 1.06474 to 1.61785. The table also indicates the Sh increases from 0.06474 to 0.61785. The negative sign means that the CO_2 is lost to the environment at the surface of the cylinder.

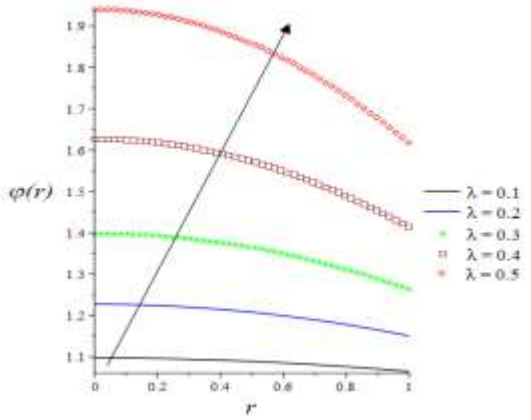

Fig. 4: λ effect on CO_2 emission

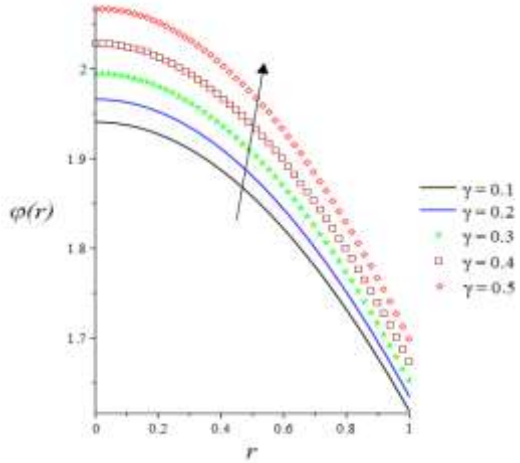

Fig. 5: γ effect on CO_2 emission

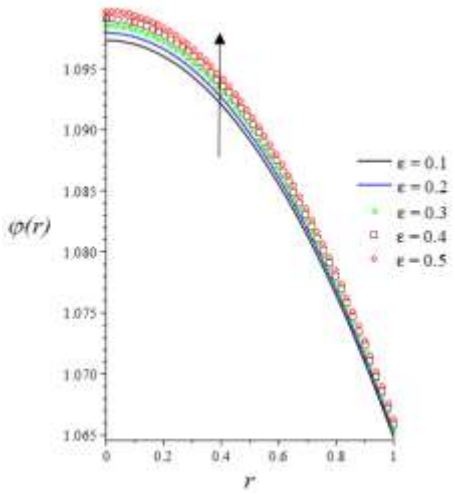

Fig. 6: ε effect on CO_2 emission

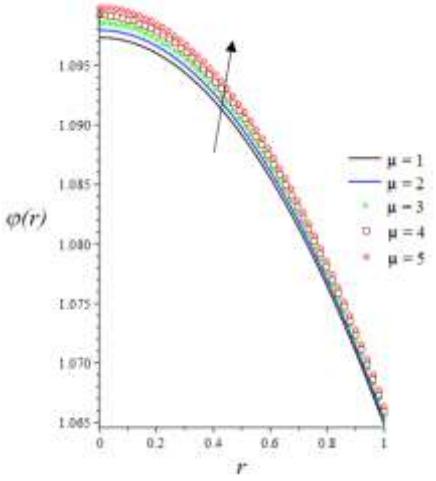

Fig. 9: μ effect on CO_2 emission

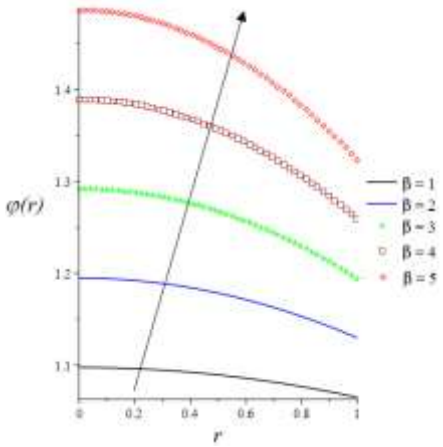

Fig. 7: β effect on CO_2 emission

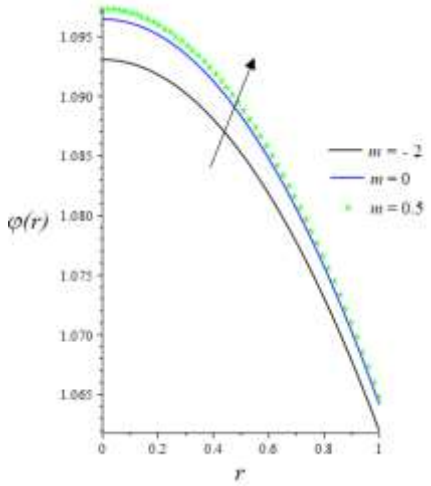

Fig. 10: m effect on CO_2 emission

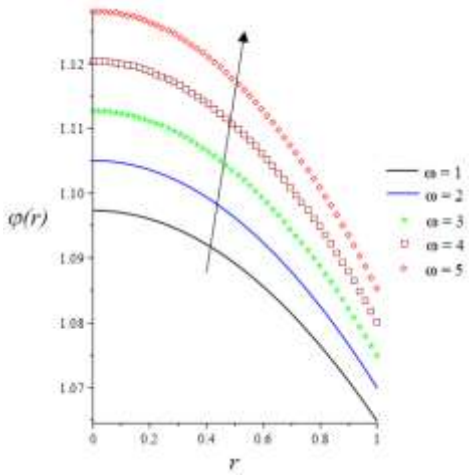

Fig. 8: ω effect on CO_2 emission

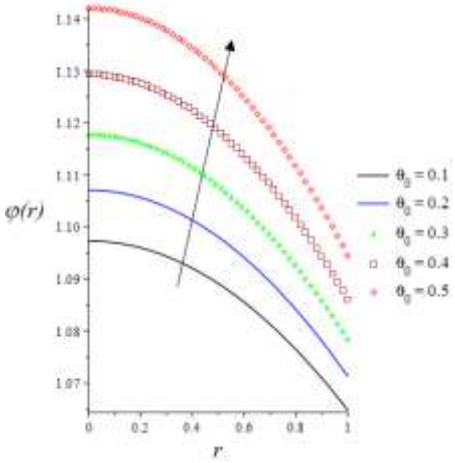

Fig. 11: θ_0 effect on CO_2 emission

Table 2: Effects of λ on CO_2 emissions (Fig. 4)

λ variation	CO_2 emissions	Sh values
0.1	1.06474	-0.06474
0.2	1.15079	-0.15079
0.3	1.26387	-0.26387
0.4	1.41344	-0.41344
0.5	1.61785	-0.61785

Table 3: γ on CO_2 emissions (Fig. 5)

γ variation	CO_2 emissions	Sh values
0.1	1.06474	-0.06474
0.2	1.06483	-0.06483
0.3	1.06493	-0.06493
0.4	1.06502	-0.06502
0.5	1.06512	-0.06512

Table 4: ε on CO_2 emissions (Fig. 6)

ε variation	CO_2 emissions	Sh values
0.1	1.06474	-0.06474
0.2	1.06514	-0.06514
0.3	1.06553	-0.06553
0.4	1.06593	-0.06593
0.5	1.06632	-0.06632

Table 5: β on CO_2 emissions (Fig. 7)

β variation	CO_2 emissions	Sh values
1	1.06474	-0.06474
2	1.12948	-0.12948
3	1.19425	-0.19425
4	1.25896	-0.25896
5	1.32369	-0.32369

Table 6: ω on CO_2 emissions (Fig. 8)

ω variation	CO_2 emissions	Sh values
1	1.06474	-0.06474
2	1.06987	-0.06987
3	1.07499	-0.07499
4	1.08012	-0.08012
5	1.08525	-0.08525

Table 7: Effects of μ on CO2 emissions (Fig. 9)

μ variation	CO_2 emissions	Sh values
1	1.06474	-0.06474
2	1.06514	-0.06514
3	1.06554	-0.06554
4	1.06595	-0.06595
5	1.06636	-0.06636

Table 8: m on CO_2 emissions (Fig. 10)

m variation	CO_2 emissions	Sh values
-2	1.06194	-0.06194
0	1.06416	-0.06416
0.5	1.06474	-0.06474

Table 9: θ_0 on CO_2 emissions (Fig. 11)

θ_0 variation	CO_2 emissions	Sh values
0.1	1.06474	-0.06474
0.2	1.07123	-0.07123
0.3	1.07832	-0.07832
0.4	1.08605	-0.08605
0.5	1.09448	-0.09448

We now consider the kinetic parameters that were observed to lower the CO_2 emission during an exothermic chemical reaction. The parameters are ϵ, σ and α. An increase in the values of these parameters shows a decline in CO_2 emissions. The scenario is depicted in Figs. 12-14. This observation also confirms that the emissions of CO_2 are very high in materials that combust spontaneously. Figs. 12 and 14 show that the heat loss and the Biot number parameters have a lesser effect on the retardation of CO_2 emission as compared to the CO_2 Biot number, illustrated in Fig. 13. Tables 10-12 confirm also what Figs. 12-14 demonstrate. These parameters are helpful to the environment because the discouragement of CO_2 emission also means a lesser heat emission to the environment to reduce the fast-growing climate change that has adversely affected the weather globally.

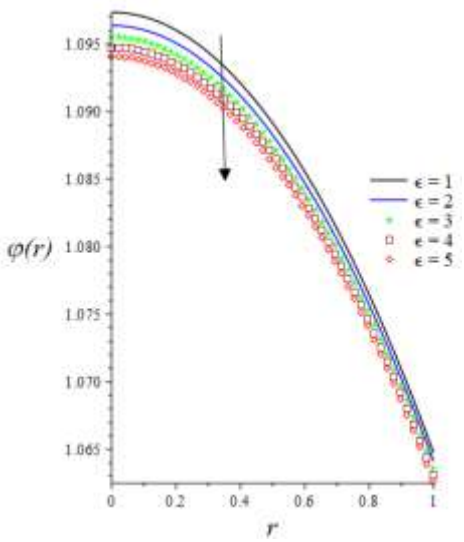

Fig. 12: ϵ effect on CO_2 emission

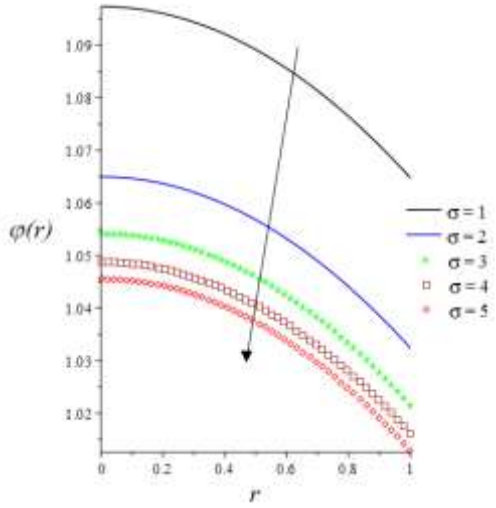

Fig. 13: σ effect on CO_2 emission

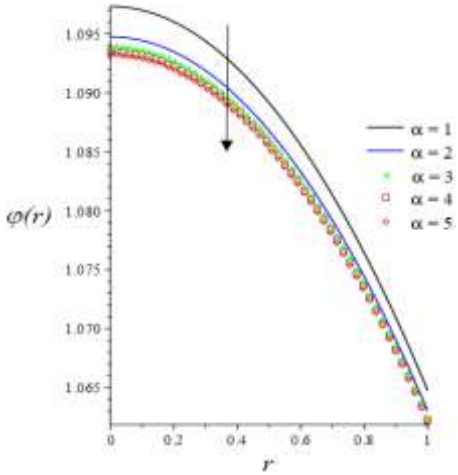

Fig. 14: α effect on CO_2 emission

Table 10: ϵ on CO_2 emissions (Fig. 12)

ϵ variation	CO_2 emissions	Sh values
1	1.06474	-0.06474
2	1.06411	-0.06411
3	1.06356	-0.06356
4	1.06308	-0.06308
5	1.06264	-0.06264

Table 11: σ on CO_2 emissions (Fig. 13)

σ variation	CO_2 emissions	Sh values
0.1	1.06474	-0.06474
0.2	1.03237	-0.06474
0.3	1.02158	-0.06474
0.4	1.01618	-0.06474
0.5	1.01295	-0.06474

Table 12: α on CO_2 emissions (Fig. 14)

α variation	CO_2 emissions	Sh values
1	1.06474	-0.06474
2	1.06302	-0.06302
3	1.06247	-0.06247
4	1.06219	-0.06219
5	1.06202	-0.06202

5 Conclusion

In this study, the analysis of CO_2 emission in a stockpile of reactive materials modeled in a cylindrical domain was considered. The kinetic parameters embedded within the differential equation governing the problem were used to bring an understanding of the CO_2 analysis process. Maple software was used to give the numerical solutions. It was found that the parameters $\lambda, \gamma, \varepsilon, \beta, \omega, \mu, m,$ and θ_0 enhance the emission of CO_2 during an exothermic chemical reaction. These parameters are not friendly to the environment because the CO_2 emissions have contributed much to climate change. On the other hand, the parameters such as ϵ, σ and α were found to reduce the CO_2 emission during a combustion process. The lessening of CO_2 emission is helpful to reduce climate change. The mathematical approach to this study allowed the CO_2 analysis in a quicker and cheaper manner as compared to the experimental one. This study can be extended to a situation where the stockpile is modeled in a spherical domain.

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Contribution of individual authors to the creation of a scientific article (ghostwriting policy)

RS Lebelo, SO Adesanya carried out the conceptualization, simulation, the overall writing, language editing and plagiarism checking.
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