Analysis of CO₂ Emission, O₂ Depletion and Thermal Stability in a Convective and Radiating Reactive Slab

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Abstract

In this article, we investigate the effects of convective and radiative heat loss on CO₂ emission, O₂ depletion and thermal stability in a stockpile of combustible material. A rectangular slab model is applied to carry out the investigation. The heat generated in a reactive slab is as a result of exothermic chemical reaction in which O₂ is a reactive species and CO₂ and heat are products. It is assumed that the surfaces of the slab lose heat by convection and radiation with the ambient. The nonlinear differential equations governing the problem are solved numerically using Runge-Kutta-Fehlberg method coupled with shooting technique. The results are presented graphically and discussed quantitatively to show the effects of various thermo-physical parameters on the temperature field, CO₂ emission and O₂ depletion. Thermo-physical parameters (processes) that reduce CO₂ emission and encourage thermal stability in exothermic chemical reactions, to reduce climate change and global warming, were identified.

Keywords: Reactive slab, CO₂ emission, O₂ depletion, convective heat loss, thermal radiation, numerical simulation technique.
INTRODUCTION

Spontaneous generation of heat in a stockpile is due to exothermic chemical reaction of combustible material within it [1, 2]. Combustible reactive material refers to hydrocarbon materials, such as plastic, sawdust, paper, just to mention few, making up the stockpile, and spontaneous reaction occurs immediately when O2 within the stockpile reacts with the material. In this study, rectangular slab model was used to study the combustion process within a stockpile of combustible material. This process of spontaneous combustion within a reactive slab has a wide range of industrial applications in the fields of solids combustion, heavy oil recovery, incineration of waste material, design of internal combustion engines and automobile exhaust system [3], to mention just a few. One of the studies has shown that exothermic chemical reaction taking place in a reactive slab may result in up to 80% emission of CO2, which contributes to global warming and climate change [4].

It should be noted too that the exothermic reaction due to reaction of hydrocarbon material with O2 within a reactive slab, also results in heat production which brings about a temperature rise in the slab [5]. On the other hand, it is possible that the rate of heat generation as a result of exothermic chemical reaction within a slab may exceed the rate of heat loss to the immediate cool environment, and this may lead to thermal explosion. This phenomenon is known as thermal criticality [6]. Thermal criticality is helpful in combustion theory to provide a safe storage criterion for materials that can easily undergo exothermic reaction [6–8].

Various studies have been carried out on thermal stability characteristics of a reacting slab, and these were done with or without reactant consumption using one-step decomposition kinetics [9–10]. In the current study, reactant consumption was taken into consideration and the complicated chemistry due to exothermic chemical reaction taking place in a reactive slab was tackled by considering one-step decomposition kinetics [11]. This consideration is helpful because the combustion reaction mechanism is very complicated and includes many radicals, especially of large hydrocarbons [12]. In addition to this, the complicated nature of exothermic reactions gives rise to nonlinear short-lived interactions involving reacting species and products diffusion, heat conduction and chemical reactions, and furthermore, these interactions lead to steep concentration and temperature gradients [13,14]. In this regard, a detailed review of chemical kinetic models for the reaction of hydrocarbons with O2 in combustible materials is provided in [15].

However, to the best of our knowledge, no or very few studies have been carried out on the effects of convective and radiation heat loss on CO2 emission, O2 depletion and thermal stability criteria for a reactive slab of combustible materials. The objective in the research on which this article is based, was to investigate the effects of heat loss due to convection and radiation on CO2 emission, O2 depletion and thermal stability in a
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stockpile of reactive combustible materials. The nonlinear differential equations governing the problem are presented in section 2, and then solved numerically using the Runge-Kutta-Fehlberg method coupled with shooting technique. Maple software was used in this case to solve the nonlinear differential equations. The results are illustrated graphically and discussed quantitatively with respect to various thermo-physical parameters embedded in the system.

MATHEMATICAL MODEL

A rectangular slab of combustible material with constant thermal conductivity $k$, and surface emissivity $\varepsilon$, is considered in this article. It is assumed that the slab is undergoing an $n^{th}$ order oxidation chemical reaction. A one-step finite rate irreversible chemical kinetics mechanism between the material and the oxygen of the air is assumed and expressed as follows:

\[ C_iH_j + \left( i + \frac{j}{4} \right) O_2 \rightarrow iCO_2 + \left( \frac{j}{2} \right) H_2O + \text{heat}. \]

Heat loss as a result of radiation at the material surface to the surrounding environment is given by $q = \varepsilon \sigma (T^4 - T_0^4)$, according to Stefan-Boltzmann’s law. Convective heat loss at the surface of the slab follows Newton’s law of cooling and it is generally indicated as $-\frac{h}{k} [T - T_\infty]$. Convection and radiation are considered to take place in the $\bar{y}$ direction. Figure 1 below illustrates the geometry of the problem. Consider convective heat loss above and below the slab, and radiative heat loss, which is assumed to occur solely on the upper surface of the slab where the medium is mainly air.

![Figure 1: Geometry of the problem](image)
Following [4,9,15,16,17], nonlinear governing differential equations for heat and mass transfer problem in the presence of convection, thermal radiation, CO2 emission and O2 depletion are written as:

\[ k \frac{d^2 T}{dy^2} + Q A \left( \frac{K_T}{vl} \right)^m C^n \exp \left( \frac{-E}{RT} \right) - \varepsilon \sigma (T^4 - T_\infty^4) = 0, \]  

(1)

\[ D \frac{d^2 C}{dy^2} - A \left( \frac{K_T}{vl} \right)^m C^n \exp \left( \frac{-E}{RT} \right) = 0, \]  

(2)

\[ \gamma \frac{d^2 P}{dy^2} + A \left( \frac{K_T}{vl} \right)^m C^n \exp \left( \frac{-E}{RT} \right) = 0, \]  

(3)

with boundary conditions at the bottom and the top of the reactive slab respectively as:

\[ \bar{y} = 0, \quad k \frac{dT}{d\bar{y}} = h_1 (T - T_\infty), \quad C = C_w, \quad P = P_w, \]  

(4)

\[ \bar{y} = a, \quad -k \frac{dT}{d\bar{y}} = h_2 (T - T_\infty), \quad C = C_w, \quad P = P_w. \]  

(5)

\( T \) is the slab’s absolute temperature and \( C \) the O2 concentration. The term \( P \) represents CO2 concentration while \( T_\infty \) the ambient temperature and \( C_w \) is the O2 concentration at the slab surface. The CO2 concentration at the slab surface is denoted by \( P_w \), \( k \) is the thermal conductivity of the reacting slab and \( \varepsilon \) the slab’s emissivity (0 < \( \varepsilon < 1 \)). Here, \( \sigma \) is Stefan-Boltzmann constant (5.6703 \times 10^{-8} \text{W/m}^2\text{K}^4) while \( D \) is diffusivity of O2 in the slab and \( \gamma \) the diffusivity of CO2 in the slab. The term \( Q \) is the heat of reaction, \( A \) the rate constant, \( E \) the activation energy, \( R \) the universal gas constant and \( l \) the Planck’s number. We have that \( \nu \) represents the vibration frequency, \( K \) the Boltzmann constant and \( \bar{y} \) the distance measured vertically. Again, \( h_1 \) is the heat transfer coefficient at the lower surface of the slab, \( h_2 \) the heat transfer coefficient at the upper surface of the slab, while \( n \) is the order of exothermic chemical reaction, and \( m \) the numerical exponent such that \( m \in \{-2,0,0.5\} \). The three values taken by the parameter \( m \) represent, respectively, the numerical exponent for sensitized (kinetics facilitated by substance other than catalyst), Arrhenius and Bimolecular kinetics [1,2,4,15]. The boundary conditions (4) and (5) describe the temperature conditions due to convective heat loss at the base and the top of the reactive slab respectively, and radiative heat loss is assumed to take place only at the upper surface of the slab.
The following dimensionless parameters are introduced to eq. (1) – (5):

\[
\theta = \frac{E(T-T_\infty)}{RT_\infty^2}, \quad \Phi = \frac{C}{C_w}, \quad \Psi = \frac{P}{P_w}, \quad Bi_2 = \frac{ah_2}{k}
\]

\[
\beta_1 = \frac{kRT_\infty}{QEDC_w}, \quad \beta_2 = \frac{kRT_\infty}{QEFP_w}, \quad Bi_1 = \frac{ah_1}{k}
\]

\[
\lambda = \left(\frac{KT_\infty}{vI}\right)^m \frac{QAEa^2(C_w)^n}{kRT_\infty^2} \exp\left(-\frac{E}{RT_\infty}\right),
\]

\[
y = \frac{y}{a}, \quad \mu = \frac{RT_\infty}{E}, \quad Ra = \frac{\xi\sigma a^2T_\infty^2}{kR}.
\]

(6)

Eq. (1) – (5) take the dimensionless form

\[
\frac{d^2\theta}{dy^2} + \lambda(1+\mu\theta)^m \Phi^n \exp\left(\frac{\theta}{1+\mu\theta}\right) - Ra((\mu\theta + 1)^4 - 1) = 0,
\]

(7)

\[
\frac{d^2\Phi}{dy^2} - \lambda\beta_1 (1+\mu\theta)^m \Phi^n \exp\left(\frac{\theta}{1+\mu\theta}\right) = 0,
\]

(8)

\[
\frac{d^2\Psi}{dy^2} + \lambda\beta_2 (1+\mu\theta)^m \Phi^n \exp\left(\frac{\theta}{1+\mu\theta}\right) = 0,
\]

(9)

\[
y = 0, \quad \frac{d\theta}{dy} = Bi_1 \theta, \quad \Phi = 1, \quad \Psi = 1,
\]

(10)

\[
y = 1, \quad \frac{d\theta}{dy} = -Bi_2 \theta, \quad \Phi = 1, \quad \Psi = 1.
\]

(11)

Here, \(\lambda\) is the Frank-Kamenetskii parameter and \(\mu\) the activation energy parameter. The parameter \(\beta_1\) represents O2 consumption rate, \(\beta_2\) is the CO2 emission rate parameter, \(Bi_1\) the Biot number at the slab’s lower surface, \(Bi_2\) the Biot number at the slab’s upper surface and \(Ra\) the radiation parameter. The dimensionless heat and mass transfer rates at the slab’s surface are expressed in terms of Nusselt number (\(Nu\)) and Sherwood numbers (\(Sh_1, Sh_2\)), respectively, as follows:

\[
Nu = -\frac{d\theta}{dy} \text{ (at } y = 1), \quad Sh_1 = \frac{d\Phi}{dy} \text{ (at } y = 1), \quad Sh_2 = -\frac{d\Psi}{dy} \text{ (at } y = 1)
\]

(12)

The dimensionless heat and mass transfer rates at \(y = 0\) are not indicated since radiation is assumed to take place only on the upper part of the slab. Eq. (7) – (9) and the boundary conditions (10)–(11) are solved numerically by the application of Runge-
Kutta-Fehlberg method (RKF45) coupled with shooting technique [14]. The shooting technique involves solving a boundary value problem by reducing it to an initial value problem. The process of shooting may use bisection scheme or Newton-Raphson method [18]. The error minimization is attained by using small step sizes when constructing the solutions by Runge-Kutta of order 4. The coupled RKF45 and shooting technique methods are embedded in any mathematical software, and in this article, Maple software was applied to give results graphically. From the process of numerical computation, \( Nu \), \( Sh_1 \), and \( Sh_2 \) in eq. (12) are also worked out and presented graphically too.

3. NUMERICAL ALGORITHM

Equations (7) – (11) were solved using RKF45 method coupled with shooting technique, as mentioned earlier. The algorithm gives results to expected accuracy. The following algebraic procedure is used, where, \( \theta = x_1 \), \( \theta' = x_2 \), \( \Phi = x_3 \), \( \Phi' = x_4 \), \( \Psi = x_5 \), \( \Psi' = x_6 \). It becomes possible to transform equations (7) – (11) to first order differential equations as follows:

\[
\begin{align*}
\dot{x}_1' &= x_2 \\
\dot{x}_2' &= -\lambda (1 + \mu x_1)^m (x_3)^n \exp\left(\frac{x_1}{1+\mu x_1}\right) - Ra[(\mu x_1 + 1)^4 - 1] \\
\dot{x}_3' &= x_4 \\
\dot{x}_4' &= \lambda (1 + \mu x_1)^m (x_3)^n \exp\left(\frac{x_1}{1+\mu x_1}\right) \\
\dot{x}_5' &= x_6 \\
\dot{x}_6' &= -\lambda (1 + \mu x_1)^m (x_3)^n \exp\left(\frac{x_1}{1+\mu x_1}\right).
\end{align*}
\]

(13)

Equations in (13) are subject to the following boundary conditions:

\[
\begin{align*}
x_1(0) &= Bi_1 x_1, \ x_3(0) = 1, \ x_5(0) = 1, \ x_1(1) = -Bi_2 x_1, \ x_3(1) = 1, \ x_5(1) = 1
\end{align*}
\]

(14)

RESULT AND DISCUSSION

In this section, we present computational results obtained from the modelled equations in the above section graphically, and discuss the results quantitatively for various values of thermo-physical parameters embedded in the system.
Effects of thermo-physical parameter variation on slab temperature profiles:

The effects of some parameters on temperature profiles are illustrated by Figures 2 – 9. We observe from Figure 2 that the temperature increases with increasing $\lambda$. This means that increasing the rate of reaction in a reactive slab increases exothermic chemical reaction which favors increase in temperature. A different observation is shown by Figures 3 – 8 in which an increase in $Ra$, $n$, $\mu$, $Bi_1$, $Bi_2$ and $\beta$, respectively, results with a decrease on temperature profiles. These parameters are helpful to keep the temperature of the slab low and thus the thermal stability of the system is attained. Figure 6 shows that as $Bi_1$ increases, temperature profiles are lower at the bottom of the slab as compared to the top of the slab. An opposite scenario is observed in Figure 7, where an increase in $Bi_2$ shows lower temperature profiles at the upper surface of the slab as compared to the lower surface of the slab. Effect of $m$ on temperature is illustrated by Figure 9. In this case, we observe that the temperature profiles increase with increasing $m$, and that the temperature is low during sensitized ($m = -2$) and highest during Bimolecular ($m = 0.5$) reactions respectively.

![Figure 2: Effect of increasing $\lambda$ on slab temperature profiles.](image-url)
Figure 3: Effect of increasing $Ra$ on slab temperature profiles

Figure 4: Effect of increasing $n$ on slab temperature profiles
Figure 5: Effect of increasing \( \mu \) on slab temperature profiles

Figure 6: Effect of increasing \( Bi_1 \) on slab temperature profiles.
Figure 7: Effect of increasing $Bi_2$ on slab temperature profiles.

Figure 8: Effect of increasing $\beta_1$ on slab temperature profiles.
Effects of thermo-physical parameter variation on slab O2 depletion:

In this section, we consider effects of parameter variation on slab O2 depletion in a reactive slab of combustible material. The effects are illustrated in Figures 10 - 17. We observe from Figure 10 that increasing the rate of reaction \( \lambda \) increases the depletion of O2 due to accelerated exothermic chemical reaction within the slab. From Figure 11 we see an opposite scenario that increasing the radiation parameter \( Ra \), results with conservation of O2 concentration as illustrated by increase in O2 profiles, and the same situation is shown by Figure 12, where an increase in the order of reaction \( n \) results with corresponding increase in O2 profiles. An increase in \( \beta_1 \) decreases the O2 concentration within a reactive slab as shown by Figure 13. This means that more O2 is used up during the process which enhances exothermic chemical reaction. An increase in activation energy \( \mu \) shows a corresponding increase in O2 profiles as demonstrated by Figure 14. It is interesting to note that a chemical reaction with high activation energy will stimulate an exothermic reaction that will not require much of O2 that is so useful to life. Figure 15 illustrates the effect of increasing \( Bi_1 \) on slab O2 depletion profiles. We observe from the figure that as \( Bi_1 \) increases, O2 profiles also increase. From Figure 16 it is noticed also that an increase in \( Bi_2 \) shows a corresponding, but almost negligible, increase in O2 profiles, meaning that the exothermic reaction is decelerated. A decrease in O2 profiles as \( m \) increases is illustrated by Figure 17. Lesser O2 is used up during sensitized reactions as compared to both Arrhenius and Bimolecular reactions.
Figure 10: Effect of increasing $\lambda$ on slab Oxygen depletion profiles.

Figure 11: Effect of increasing $Ra$ on slab Oxygen depletion profiles
Figure 12: Effect of increasing $n$ on slab Oxygen depletion profiles

Figure 13: Effect of increasing $\beta_1$ on slab Oxygen depletion profiles.
Figure 14: Effect of increasing $\mu$ on slab Oxygen depletion profiles.

Figure 15: Effect of increasing $Bi_1$ on slab Oxygen depletion profiles.
Figure 16: Effect of increasing $Bi_2$ on slab Oxygen depletion profiles.

Figure 17: Effect of increasing $m$ on slab Oxygen depletion profiles.
Effects of thermo-physical parameter variation on slab CO\textsubscript{2} emission:

Effects of some thermo-physical parameters on CO\textsubscript{2} emission are discussed in this subsection. Figures 18 – 26 illustrate these effects. From Figure 18 we observe that an increase in the rate of reaction $\lambda$ results with an increase in CO\textsubscript{2} emission. This is due to the accelerated exothermic chemical reaction within the slab which gives out more CO\textsubscript{2} as a product. A different scenario is shown in Figures 19 and 20, where an increase in both $Ra$ and $n$, result with a decrease in CO\textsubscript{2} profiles respectively. We have seen from previous discussions that higher values of $n$ and $Ra$ help to preserve O\textsubscript{2}. The same scenario is observed in Figure 21, where CO\textsubscript{2} profiles decrease with an increase in $\beta_1$. Figure 22 shows the effect of increasing $\beta_2$ on slab CO\textsubscript{2} emission profiles. An increase in CO\textsubscript{2} emission rate parameter ($\beta_2$) shows a corresponding increase in CO\textsubscript{2} emission. Figure 23 illustrates that an increase in $\mu$, the activation energy of the system, does not favour CO\textsubscript{2} emission, after observed minimal decrease in CO\textsubscript{2} profiles. The same situation is observed in Figures 24 and 25, where an increase in both $Bi_1$, Biot number at the lower surface of the slab, and $Bi_2$, Biot number at the upper surface of the slab, respectively, show minor decreases in CO\textsubscript{2}. We should note that at this surface of the slab, both convective and radiative heat loss to the surroundings are experienced. In Figure 26 we observe effect of $m$ on CO\textsubscript{2} emission. Increasing $m$ results with minor increase in CO\textsubscript{2} profiles and the emission of CO\textsubscript{2} is highest during Bimolecular reaction.

![Figure 18: Effect of increasing $\lambda$ on slab Carbon dioxide emission profiles](image-url)
Figure 19: Effect of increasing $Ra$ on slab Carbon dioxide emission profiles.

Figure 20: Effect of increasing $n$ on slab Carbon dioxide emission profiles.
Figure 21: Effect of increasing $\beta_1$ on slab Carbon dioxide emission profiles

Figure 22: Effect of increasing $\beta_2$ on slab Carbon dioxide emission profiles
Figure 23: Effect of increasing $\mu$ on slab Carbon dioxide emission profiles

Figure 24: Effect of increasing $Bi_1$ on slab Carbon dioxide emission profiles
Effects of parameter variation on thermal criticality values or blowups:

Investigated rate of reaction ($\lambda$) variation with dimensionless heat transfer rate at the slab surface ($Nu$), for various values of some thermo-physical parameters as shown by

**Figure 25:** Effect of increasing $Bi_2$ on slab Carbon dioxide emission profiles

**Figure 26:** Effect of increasing $m$ on slab Carbon dioxide emission profiles
the Figures 27–32, is discussed in this subsection. It is important to note that results obtained for $Nu$ are qualitatively the same for both $Sh_1$ and $Sh_2$. Results are represented also in Table 1.

The effect of increasing $Ra$ on slab thermal criticality values is shown in Figure 27. It is observed that as $Ra$ is increased, $Nu$ and $\lambda$ are also increased. It is observed that blowups (explosions) occur faster at lower values of $Ra$, as $\lambda$ increases. The blowups are quicker at both lower values of $Nu$ and $\lambda$. The quickest blowups are illustrated by the shortest curves in all figures that are discussed. The longest curves show that the blowups take the longest time to occur, and therefore thermal stability is reasonably attained. It is therefore necessary to keep the $Ra$ values higher to allow thermal stability of the system. Figure 28 illustrates the effect of increasing $n$ on slab thermal criticality values. We observe the same scenario as in Figure 27, that as $n$ increases, $Nu$ also increases correspondingly with $\lambda$. The blowups also occur faster at lower values of both $\lambda$ and $Nu$. From Figure 29 the same situation as in Figure 27 and Figure 28 is observed. Thermal stability is attained by keeping higher values of $Bi_1$, $\lambda$ and $Nu$. We also observe the repetition of the process in Figure 30 and Figure 31, where both $\lambda$ and $Nu$ increase with increasing $Bi_2$ and $\mu$ respectively, and that thermal stability is attained by taking higher values of $Bi_2$ and $\mu$. A different scenario is observed in Figure 32, where $Nu$ and $\lambda$ decrease with increasing $m$ and that thermal stability is attained by keeping the lowest value of $m$ and highest values of $\lambda$ and $Nu$. Numerical values for variation of parameters discussed, and corresponding results for $\lambda$ and $Nu$, are written in Table 1 below.

Figure 27: Effect of increasing $Ra$ on slab thermal criticality values.
Figure 28: Effect of increasing $n$ on slab thermal criticality values.

Figure 29: Effect of $Bi_1$ on slab thermal criticality values.
**Figure 30:** Effect of $Bi_2$ on slab thermal criticality values.

**Figure 31:** Effect of increasing $\mu$ on slab thermal criticality values.
Figure 32: Effect of increasing $m$ on slab thermal criticality values.

Table 1: Computations showing the effects of various thermo-physical parameters on thermal criticality values, where we have that $\beta_1 = \beta_2 = 0.1$.

<table>
<thead>
<tr>
<th>$Ra$</th>
<th>$n$</th>
<th>$\mu$</th>
<th>$Bi_1$</th>
<th>$Bi_2$</th>
<th>$m$</th>
<th>$Nu$</th>
<th>$\lambda$</th>
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CONCLUSION

In this article, we looked at the analysis of CO\textsubscript{2} emission, O\textsubscript{2} depletion and thermal stability in a convective and radiative reactive slab. From the results observed, the general trend is that processes which increase both the temperature and CO\textsubscript{2} emission profiles increase the depletion of O\textsubscript{2} in a reactive slab. The thermo-physical parameters identified to lessen CO\textsubscript{2} emission in an exothermic reaction are $n$, $Bi_1$, $Bi_2$, $\beta_1$, $Ra$ and $\mu$. Thermo-physical parameters which help to achieve thermal stability, that is, explosion prevention within a stockpile of combustible material were also identified as $Ra$, $n$, $Bi_1$, $Bi_2$ and $\mu$.

The significance of the study of reactive materials in a rectangular slab may include rectangular storage of carbon containing materials such as industrial waste, sugarcane bagasse, coal, hays and wool wastes, to mention a few. The results obtained and discussed reveal the effect of storage geometry on the exothermic reaction and CO\textsubscript{2} emission in reactive materials which invariably affect the environment through the production of ozone layer. Increased production of ozone leads to climate change and global warming.

The limitation to the investigation carried out is that only theoretical approach was considered. The investigation can be extended by also consideration of experimental approach. But, the adoption of mathematical model to simulate this complicated phenomenon makes it easier to provide insight into this difficult problem. Moreover, mathematical modelling approach is a cheaper and safer way, because the experimental approach may involve hazards as a result of exothermic chemical reaction.

Differential equations that govern the problem were obtained, and the equations were solved numerically using Runge-Kutta-Fehlberg method coupled with shooting technique. Results were presented graphically and discussed accordingly. Using the same derived non-linear differential equations, the investigation can be extended to cylindrical vessels with coordinates, say, $(z, r, \theta)$ and also spherical vessels with $(r, \theta, \phi)$ as coordinates.

REFERENCES


