

Radiation and Thermal Decomposition Analysis in a Reactive Slab of Variable Thermal Conductivity.

RS Lebelo^{*1}, KC Moloi¹, CC Chitumwa¹ and SO Adesanya^{1,2}

¹Department of Education, Vaal University of Technology, Private Bag X021, Vanderbijlpark, 1911, South Africa
sollyl@vut.ac.za; conniem@vut.ac.za; chrisc@vut.ac.za.

²Department of Mathematical Sciences, College of Natural Sciences, Redeemer's University, Ede, Nigeria.
adesanyas@run.edu.ng.

Abstract

In this article, the impact of radiative heat loss in a stockpile of combustible material is investigated. The heat loss is attributed to the exothermic chemical reaction when the carbon containing material of the stockpile reacts automatically with the oxygen trapped within the stockpile. The study is modelled in a rectangular slab of thermal conductivity that varies with the temperature and loses heat to the surrounding environment by radiation. The differential equations governing the problem are solved numerically using the Runge-Kutta-Fehlberg (RKF) method coupled with the Shooting technique. The effect of each embedded kinetic parameter on the temperature, oxygen (O₂) depletion and carbon dioxide (CO₂) emission, is analyzed and the results are graphically expressed and discussed accordingly. The results show that the kinetic parameters which enhance the exothermic chemical reaction correspondingly increase the temperature and the CO₂ emission during the combustion process, and in turn, these parameters also increase the depletion of O₂.

Key words: Radiative heat loss, exothermic chemical reaction, reactive slab, thermal decomposition.

1. Introduction

Analysis of the impact of radiative heat loss on a stockpile of combustible material is considered in this article. A combustible material is the one that contains the carbon or hydrocarbon compound that readily reacts with the oxygen trapped within the reactive stockpile. An example of a reactive stockpile is a heap of coal or rubbish containing hay, cotton or wool, or a mixture thereof. The spontaneous reaction between the carbon and the oxygen results with carbon dioxide and heat as parts of the products. Progressive accumulation of heat within the stockpile, due to the exothermic chemical reaction, results in an increase in the temperature. If the temperature of the system keeps on increasing, and the heat loss to the surrounding environment is exceeded by its production due to continued exothermic chemical reaction, thermal runaway that may lead to self-ignition of the stockpile will occur [1, 2, 3]. The exothermic chemical reaction taking place within a stockpile of combustible material is of environmental importance. Previous studies brought to light that about 80% of carbon dioxide contributing to the Greenhouse effect is due to self-ignited fires from neglected stockpiles containing materials such as cotton, hay, wood, or wool, for example [4, 5]. The emission of carbon dioxide and heat from ignition processes such as coal burning including other reactive material in households and particularly industries, contributed considerably to climate change and

global warming [6, 7]. This is evidenced by the potential collapse of the Totten Glaciers due to warmth of the climate [8]. Spontaneous ignition of combustible materials that are not attended to, is one of the main causes of veld fires which are hazardous to living species and the environment at large. In another investigation, it was maintained that veld fire is still a

great challenge and cause of harm to natural resources, forests and animal habitats, including, at some point, loss of life and property [9]. The combustion process due to spontaneous reaction between combustible material and oxygen results in an extremely complicated reaction mechanism. An elaborate chemical kinetics model for the reaction mechanism involving combustible materials and oxygen is outlined in [10]. The combustion reaction mechanism is incredibly complicated and involves many radicals. Thus, to study radiative heat loss impact of the system, mathematical modelling is necessary [11]. The impact of radiative heat loss on combustible materials with constant thermal conductivity was studied in [12]. The objective of this study was to investigate the behaviors of the temperature, O₂ depletion and CO₂ emission, in a combusting stockpile of reactive materials of variable thermal conductivity, subjected to radiative heat loss. The article outlay is as follows, the methodology part is given in section 2, the mathematical modelling is performed in section 3, section 4 elaborates on the numerical method applied to solve the nonlinear differential equations governing the problem, and, the out lay of the graphical results and the discussion thereof is in section 5.

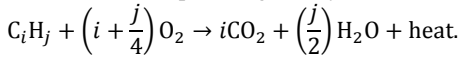
2. Methodology

The analysis of radiation and thermal decomposition in a reactive slab, is conducted theoretically with the application of mathematics to investigate the impact of radiative heat loss on the temperature, the O₂ depletion and the CO₂ emission during a combustion process. The investigation is carried out by varying the kinetic parameters with suitable arbitrary values, to understand the behavior of the temperature, O₂ depletion and CO₂ emission, during the combustion process. For example, to study the effect of the activation energy parameter (ε) in this investigation, the

following values, 0.1, 0.4, 0.7 and 1 were applied whilst other parameters were kept constant. The effect of each parameter used was investigated similarly. The partial differential equations for energy, to investigate the temperature, and for mass transfer, to investigate both the O₂ depletion and the CO₂ emission, are described under the mathematical modelling section. The equations were converted into the dimensionless state to allow a form that can be easily solved using the numerical methods, as demonstrated in equations 6. The numerical forms of the dimensionless equations are expressed under the numerical method section. The numerical algorithms to solve the nonlinear systems are embedded in numerous mathematical software, and in this investigation, Maple software was applied to solve the equations. For each parameter used, an appropriate Maple programming was drawn to give the graphical solutions to the equations. The effect of a selected parameter on the temperature, the O₂ depletion and the CO₂ emission behaviors, is depicted in graphs, as the parameter is varied. More explanation on the effects of the parameters is provided under the results and discussion section.

3. Mathematical Modelling

The exothermic chemical reaction taking place within a stockpile of combustible material is modelled in a rectangular slab. It is assumed that the slab undergoes an n^{th} order oxidation chemical reaction and the complicated reaction is simplified in a one-step finite irreversible process given by [3,4,12]



The reactive slab is also assumed to lose heat to the surrounding environment by radiation, and the heat loss is expressed as $q = \mu\sigma(T^4 - T_w^4)$, following the Stefan-Boltzmann's law. In this case μ , is the solid slab's surface emissivity such that $0 < \mu < 1$, σ is the Stefan-Boltzmann constant which is approximated at $5.6703 \times 10^{-8} W/m^2 K^4$, T is the slab's absolute temperature and T_w is the ambient temperature. The slab's material is of thermal conductivity k , that varies with the temperature at $t > 0$ and it is expressed as $k = \tau e^{b(T-T_w)}$, where τ is the material thermal conductivity at the ambient temperature T_w and b is the thermal conductivity variation parameter. The geometry of the problem is given by Fig. 1 below.

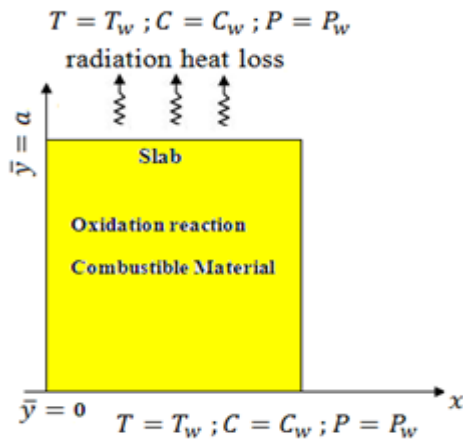


Fig. 1: The Geometry of the Problem

Fol governing the problem are:

$$k \frac{d^2 T}{dy^2} + QA \left(\frac{KT}{vl}\right)^m C^n \exp\left(-\frac{E}{RT}\right) - \mu\sigma(T^4 - T_w^4) = 0, \quad (1)$$

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

$$\gamma \frac{d^2 P}{dy^2} + A \left(\frac{KT}{vl}\right)^m C^n \exp\left(-\frac{E}{RT}\right) = 0, \quad (3)$$

with the boundary conditions:

$$\bar{y} = 0, \quad T = T_w, \quad C = C_w, \quad P = P_w, \quad (4)$$

$$\bar{y} = a, \quad T = T_w, \quad C = C_w, \quad P = P_w. \quad (5)$$

Here, C is the O₂ concentration, P is the CO₂ emission concentration, C_w is the O₂ concentration at the slab surface, P_w is the CO₂ concentration at the slab surface, D is the diffusivity of O₂ in the slab, γ is the diffusivity of CO₂ in the slab, Q is the heat of reaction, A is the rate constant, E is the activation energy, R is the universal gas constant, l is the Planck number, v is the vibration frequency, K is the Boltzmann constant, n is the order of exothermic chemical reaction, and m is the numerical exponent such that $m = -2$ is for Sensitized (laser induced) kinetics, $m = 0$ represents Arrhenius kinetics and $m = 0.5$ is for Bimolecular kinetics, following [3,4,12]. The following dimensionless parameters were introduced to equations (1) – (5)

$$\theta = \frac{E(T-T_w)}{RT_w^2}, \quad \Phi = \frac{C}{C_w}, \quad \Psi = \frac{P}{P_w}, \quad \beta = \frac{bRT_w^2}{E}, \quad \beta_1 = \frac{kRT_w^2}{QEDC_w},$$

$$\beta_2 = \frac{kRT_w^2}{QE\gamma P_w}, \quad \lambda = \left(\frac{KT_w}{vl}\right)^m \frac{QAEa^2(C_w)^n}{kRT_w^2} \exp\left(-\frac{E}{RT_w}\right), \quad y = \frac{\bar{y}}{a}, \quad \varepsilon = \frac{RT_w}{E}, \quad Ra = \frac{\mu\sigma Ea^2 T_w^4}{kR}. \quad (6)$$

Equations (1) – (5) take the dimensionless form

$$\frac{d^2 \theta}{dy^2} + \beta \left(\frac{d\theta}{dy}\right)^2 + \lambda(1 + \varepsilon\theta)^m \Phi^n e^{\theta/(1+\varepsilon\theta)} e^{-\beta\theta} - Ra[(\varepsilon\theta + 1)^4 - 1]e^{-\beta\theta} = 0, \quad (7)$$

$$\frac{d^2 \Phi}{dy^2} - \lambda\beta_1(1 + \varepsilon\theta)^m \Phi^n e^{\theta/(1+\varepsilon\theta)} e^{-\beta\theta} = 0, \quad (8)$$

$$\frac{d^2 \Psi}{dy^2} + \lambda\beta_2(1 + \varepsilon\theta)^m \Phi^n e^{\theta/(1+\varepsilon\theta)} e^{-\beta\theta} = 0, \quad (9)$$

$$y = 0, \quad \theta = 0, \quad \Phi = 1, \quad \Psi = 1, \quad (10)$$

$$y = 1, \quad \theta = 0, \quad \Phi = 1, \quad \Psi = 1, \quad (11)$$

where λ is the Frank-Kamenetski parameter, ε is the activation energy parameter, β is the variable thermal conductivity parameter, β_1 is the O₂ consumption rate parameter, β_2 is the CO₂ emission rate parameter, and, Ra is the radiation parameter.

4. Numerical Method

The set of equations (7) – (9) together with the boundary conditions (10) – (11) were solved numerically using the Runge-Kutta-Fehlberg method coupled with the Shooting technique [9]. The following is the numerical algorithm used to convert the second order differential equations into the first order form, where we consider:

$\theta = s_1, \theta' = s_2, \Phi = s_3, \Phi' = s_4, \Psi = s_5, \Psi' = s_6$. It follows that equations (6) – (11) are transformed into first order differential equations as follows:

$$s'_1 = s_2$$

$$s'_2 = -\lambda(1 + \varepsilon s_1)^m (s_3)^n e^{s_1/(1+\varepsilon s_1)} e^{-\lambda s_1} - Ra[(\varepsilon s_1 + 1)^4 - 1]e^{-\beta s_1}$$

$$s'_3 = s_4$$

$$s'_4 = \lambda(1 + \varepsilon s_1)^m (s_3)^n e^{s_1/(1+\varepsilon s_1)} e^{-\lambda s_1} \quad (12)$$

$$s'_5 = s_6$$

$$s'_6 = -\lambda(1 + \varepsilon s_1)^m (s_3)^n e^{s_1/(1+\varepsilon s_1)} e^{-\lambda s_1}, \quad (13)$$

subject to the initial conditions

$$s_1(0) = 0, \quad s_3(0) = 1, \quad s_5(0) = 1, \quad s_1(1) = 0, \quad s_3(1) = 1, \quad s_5(1) = 1 \quad (14)$$

The Shooting technique, coupled with the RKF45 gives the results to expected accuracy.

5. Results and Discussion

In this section, selected thermo-physical parameters are varied to analyse their effects on the temperature, O₂ depletion and CO₂ emission, during the combustion process. The effects of the thermo-physical parameters analysed are depicted graphically and discussed. For this purpose, the following parameters were selected, $\lambda, m, n, Ra, \varepsilon, \beta, \beta_1$ and β_2 . The following parameter values were used: $\lambda = 1, m = 0.5, n = 1, Ra = 1, \beta = 0.1, \beta_1 = 0.1, \beta_2 = 0.1, \varepsilon = 0.1$. The value of $\varepsilon = 10$ was applied only in Figs. 7, 12 and 17, for convenience.

5.1 Effects of Some Kinetic Parameters on Temperature

Figs. 2 – 7 show the effects of the parameters $\lambda, n, \varepsilon, Ra, \beta$ and m , on the temperature of the system. We observe from Fig. 2 that the temperature profiles increase as the rate of reaction parameter (λ), is increased. An increase in λ indicates the acceleration of the exothermic chemical reaction, which facilitates the release of heat within the reactive slab, hence the increase in the temperature profiles. The same scenario is observed in Fig. 7 where the effect of m on the temperature is illustrated. We observe that the

exothermic chemical reaction rate is faster in the bimolecular type of chemical reaction ($m = 0.5$) followed by that of the Arrhenius type ($m = 0$) and then lastly, the sensitized ($m = -2$) kinetics. This is confirmed by the highest level of the temperature profile for $m = 0.5$. These parameters accelerate the exothermic chemical reaction in a stockpile of reactive materials. We see a different scenario in Figs. 3, 4, 5 and 6, where an increase in the parameters n, ε, Ra and β , show a decrease in the temperature profiles of the system. Fig. 3 illustrates the effect of n (reaction order) on the temperature of the system. The decline in the temperature profiles implies that the highest order of the oxidation chemical reaction, delays the point of thermal ignition. The effect of the activation energy parameter (ε) on the temperature is illustrated in Fig. 4. An increase in ε with a decrease in the temperature, imply that the activation of the slab is very low and thus, the tendency for the slab to be volatile is reduced. Fig. 5 depicts the effect of Ra (radiation parameter) on the temperature. The increase in Ra indicates the accelerated loss of heat to the environment due to radiation. This increase leads to the delay in the development of thermal runaway of the reactive slab. In Fig. 6, the effect of the variable thermal conductivity parameter (β) on the temperature is illustrated. The increase in β also indicates the slowing down of the exothermic chemical reaction, as illustrated by the decline in the temperature profiles.

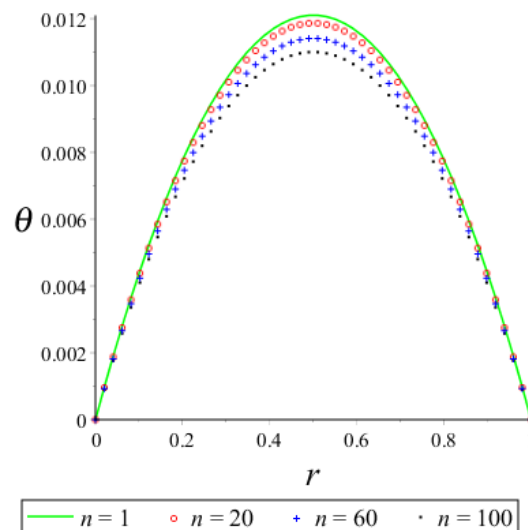


Fig. 2: λ variation with temperature

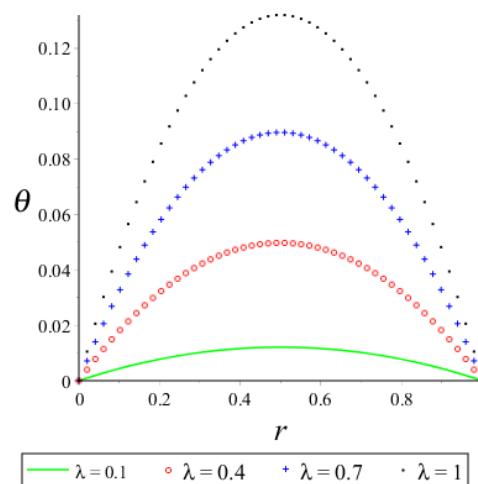


Fig. 3: n variation with temperature

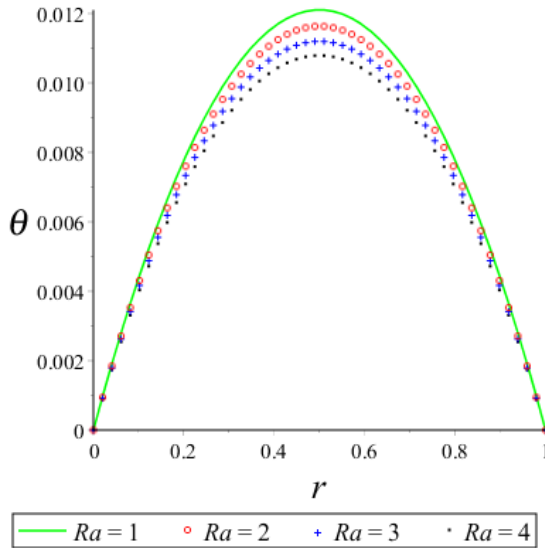


Fig. 4: ε variation with temperature

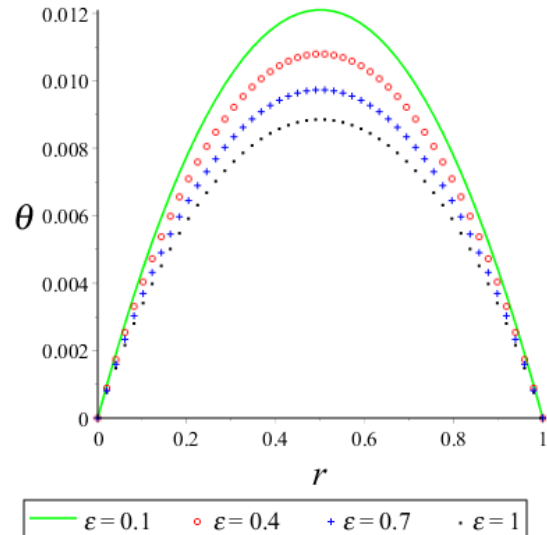


Fig. 5: Ra variation with temperature

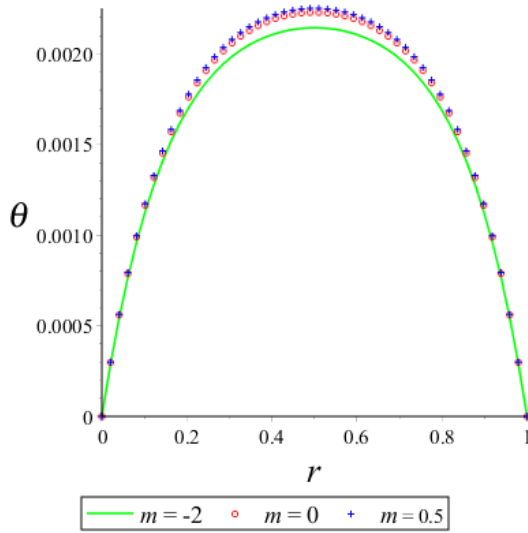


Fig. 7: m variation with temperature

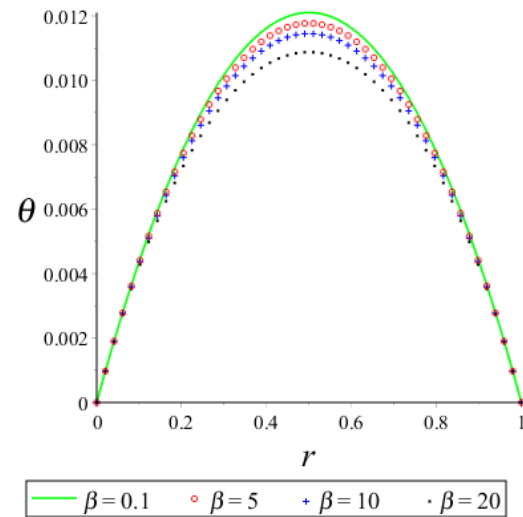


Fig. 6: β variation with temperature

5.2 Effects of Some Kinetic Parameters on O2 Depletion

We observe in Figs. 8 – 12 the effects of $\lambda, n, \beta_1, \beta$ and m on the O2 depletion within a reactive stockpile. Figs. 8, 10 and 12, show that the O2 depletion increases as λ, β_1 (O2 consumption rate parameter) and m are increased. The increased rate of O2 depletion indicates that the exothermic

chemical reaction is accelerated, and the temperature and the CO2 emission are also increased. This is not good for the environment because much of the O2 necessary for good living is consumed. Figs. 9 and 11, show that the O2 depletion of the system is reduced since the profiles of O2 in these cases increase, as the parameter n and β are increased. This situation favors the conservation of the O2 by reducing the exothermic chemical reaction rate.

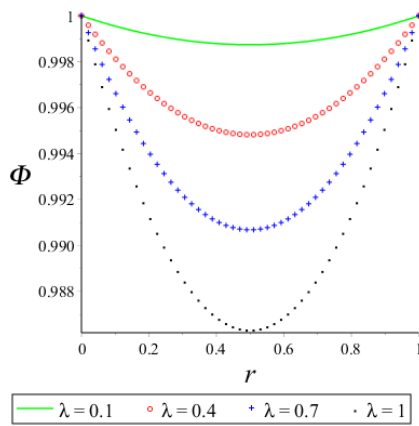


Fig. 8: λ variation with O_2 depletion

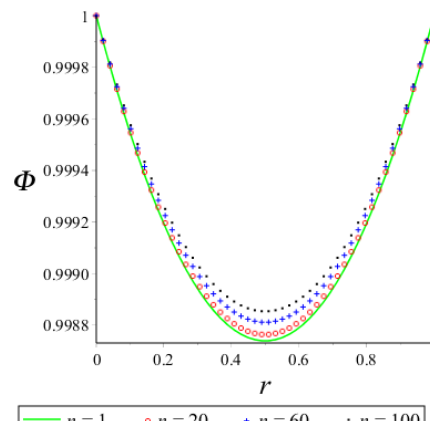


Fig. 9: n variation with O_2 depletion

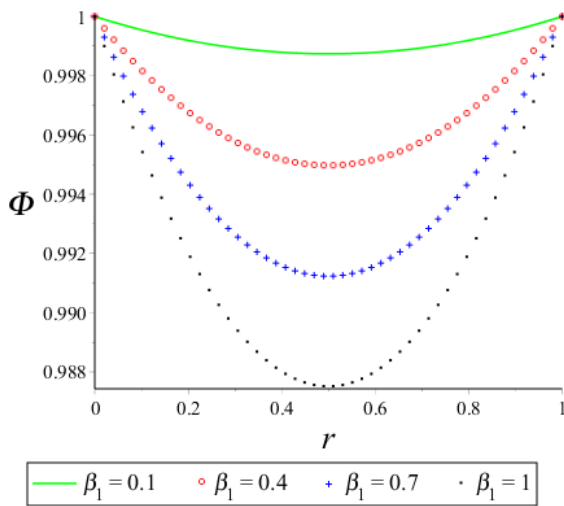


Fig. 10: β_1 variation with O_2 depletion

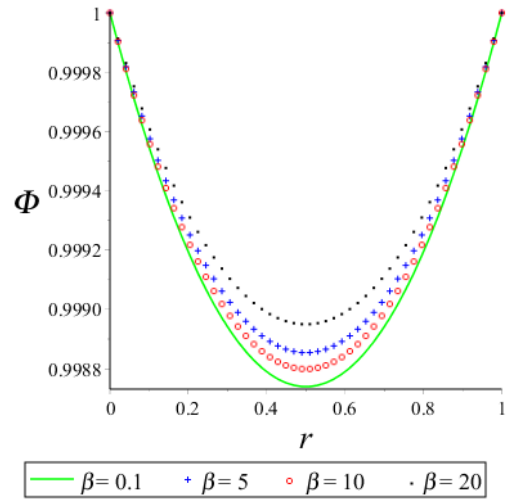


Fig. 11: β variation with O_2 depletion

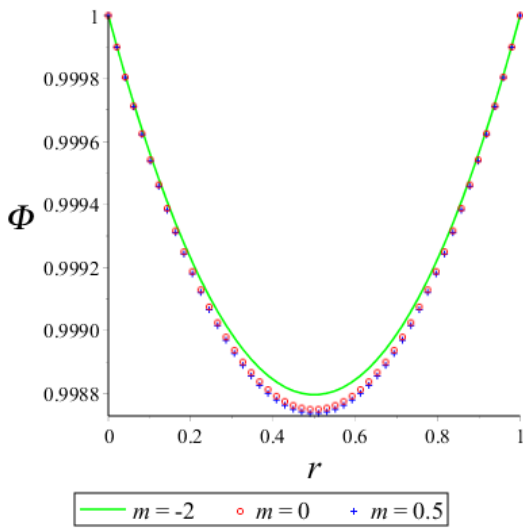


Fig. 12: m variation with O_2 depletion

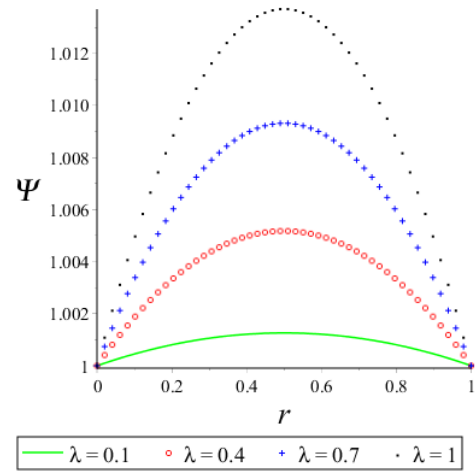


Fig. 13: λ variation with CO_2 depletion

5.3 Effects of Some Parameters on CO₂ Emission

In this subsection, we look at the effects of the parameters λ , n , β_2 , β and m on the CO₂ emission process of the system. We observe the effects in Figs. 13 – 17. In Fig. 13, 15 and 17 we see that the CO₂ profiles increase as the parameters λ , β_2 and m are increased. These parameters enhance the exothermic chemical reaction to take place resulting with more combustion and CO₂ emission. This is not beneficial for the environment, because more emission of the Greenhouse gas results in global warming and climate change. A different scenario is observed in Figs. 14 and 16, where the increase in n and β results in a decrease in CO₂ profiles. These parameters retard the exothermic chemical reaction, and this means that less CO₂ is emitted.

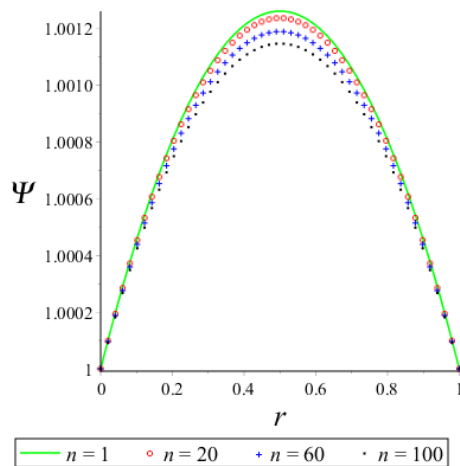


Fig. 14: n variation with CO_2 depletion

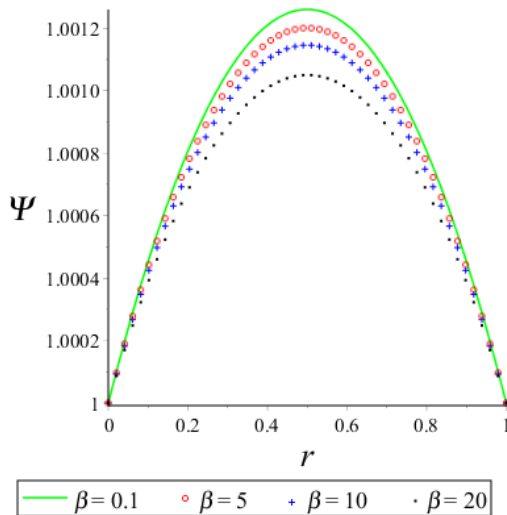


Fig. 16: β variation with CO_2 depletion

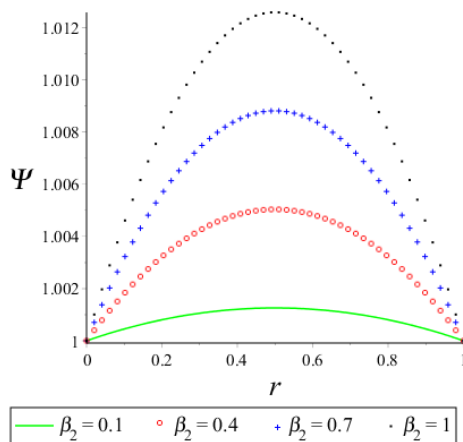


Fig. 15: β_2 variation with CO_2 depletion

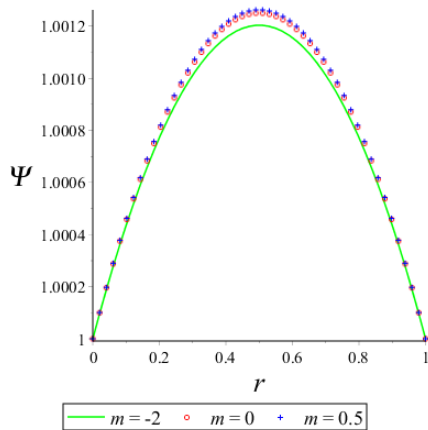


Fig. 17: m variation with CO_2 depletion

6. Conclusion

The study of the impact of radiation on combustion process in a stockpile of reactive materials with variable thermal conductivity was conducted in this article. The study was modelled in a rectangular slab. It was observed that some kinetic parameters encourage the exothermic chemical reaction to take place and therefore the system's temperature and CO_2 emission are increased, which is not good for the environment. The kinetic parameters that increase the temperature and the CO_2 emission, do also accelerate the depletion of O_2 . These parameters were found to be λ, m, β_1 and β_2 . It was also

discovered that the following kinetic parameters ε, Ra and β reduce the rate of the exothermic chemical reaction within a stockpile of reactive materials. These kinetic parameters are good for the environment because they reduce the depletion of O_2 , temperature increase, and the CO_2 emission. The significance of this study is to provide a cheaper way of understanding the combustion process in stockpiles of reactive materials, using the application of mathematics. This study can be extended to incomplete combustion processes where the effects of kinetic parameters on the carbon monoxide emission can be studied too.

About The Authors

First Author Ramoshweu S. Lebelo, PhD., researcher of the "Heat transfer analysis in combustible materials." The author's major is computational fluid dynamics.

Second Author Kholeka C. Moloi, D. Ed., senior professor of Educational Studies.

Third Author Chemunondirwa C. Chitumwa, PhD., senior lecturer in Physics.

Fourth Author Samuel O. Adesanya, PhD., senior lecturer in Mathematics.

CONFLICT OF INTEREST

The author confirms that this article content has no conflict of interest.

Acknowledgements

The authors would like to thank the Vaal University of Technology for availing the facilities to produce this work.

References

- [1] R. S. Lebelo, Thermal Stability Investigation in a Reactive Sphere of Combustible Material, *Advances in Mathematical Physics*, Vol. 2016, Article ID 9384541, 6 pages, 2016.
- [2] R. S. Lebelo, Transient Heat Analysis in a Spherical Domain of Combustible Material, *Journal of Communication and Computer*, Vol. 13(2016), pp. 159-163, 2016.
- [3] R. S. Lebelo and O. D. Makinde, Numerical investigation of CO_2 emission and thermal stability of a convective and radiative stockpile of reactive material in a cylindrical pipe, *Advances in Mechanical Engineering*, Vol. 7, no. 12, pp. 1-11, 2015.
- [4] R. S. Lebelo, Numerical investigation of CO_2 emission and thermal stability of a convective and radiative stockpile of reactive material in a cylindrical pipe of variable thermal conductivity, in *Proceedings of the AIP Conference Proceedings*, vol. 1621, pp. 60-68, 2014.
- [5] O. D. Makinde, T. Chinyoka and R. S. Lebelo, Numerical investigation into CO_2 emission, O_2 depletion and thermal decomposition in a reacting slab," *Math Probl Eng*. Vol. 2011; Article ID 208426, 19 pages, 2011.
- [6] A. Shah, Climate Change and Global Warming, *Global Issues*. Available at <http://www.globalissues.org/issue/178/climate-change-and-global-warming> [02 Feb. 2015].
- [7] E. Moll, Greenhouse Effect on the Climate & Global Warming, www.greenliving.nationalgeographic.com [26 February 2011]
- [8] A. R. A. Aitken, etal, Repeated large-scale retreat and advances of Totten Glacier indicated by inland bed erosion, *Nature* 533, pp. 385-389, 2016.
- [9] L. Mzapi, Veld Fires threaten the environment, <http://www.sundaymail.co.zw> [17 April 2016]
- [10] J. M. Simmie, Detailed chemical kinetic models for the combustion of hydrocarbon fuels, *Progress in Energy and Combustion Science*, Vol. 29, no. 6, pp. 599-634, 2003.
- [11] O. D. Makinde, Hermite-Pade' approach to thermal stability of reacting masses in a slab with asymmetric convective cooling, *J Frankl Inst.*; Vol. 349, pp. 957-965, 2012.
- [12] R. S. Lebelo and O. D. Makinde, Modelling the impact of radiative heat loss on co_2 emission, O_2 depletion and thermal stability in a reactive slab, *IJST, Transactions of Mechanical Engineering*, Vol. 39, No. M2, pp 351-365, 2015