

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

Annord Mwapinga

Department of Natural Sciences and Information Technology
Mwenge Catholic University
P.O. Box 1226 Moshi-Tanzania
Email: annord.mwapinga@mwecau.ac.tz

Received 11 November 2024; accepted 21 December 2024

Abstract. A mathematical formulation and numerical investigation of oxygen depletion, carbon dioxide emission and heat generation is studied. Models formulated were assumed to be under unsteady conditions. The explicit finite difference scheme was used to tackle the problem. The simulation was done using MATLAB software. The model parameters were varied to see the effect. The study found that increasing the Frank-Kamenetskii parameter reduces the amount of oxygen. Besides, the effect of increasing activation energy on oxygen was observed to gradually slow down the consumption of oxygen gas. Modelling the Stockpile combustion is very important to addressing its contribution in climate change. Such models can be used to predict the depletion of oxygen gas and emission of carbon dioxide.

Keywords: Modeling, stockpile, combustion, oxidation reaction, finite difference method

AMS Mathematics Subject Classification (2010): 00A71

1. Introduction

In the context of waste management, industries, hospitals, cities and municipals store some of the radioactive material in some special areas. Over time, and on a gradual basis, this contributes to global warming because when such reactive materials are stored for some time, the self-heating takes place due to oxidation reactions. This gradually leads to the emission of carbon dioxide into the atmosphere. It is important to note that spontaneous combustion happens when a material heats up to its ignition point without any external spark or flame. This can occur in substances like coal, hay, or compost, where chemical reactions or microbial processes generate heat that the material cannot release quickly enough. For instance, coal contains sulfur, which can undergo oxidation reactions that release heat, leading to a gradual buildup of temperature. If the material is not adequately ventilated, the heat can accumulate to the point of ignition.

The climate change has some dangers to our environment. Besides, there is a high risk for food security and nutrition which are linked to ongoing change of the climate [1], [2],[3]. Mathematical modelling of the Stockpile combustion is very important to

Annord Mwapinga

addressing its contribution in climate change. Such models can be used to predict the depletion of oxygen gas and emission of carbon dioxide. Research on the transient heating of combustible materials caused by exothermic oxidation reactions is crucial and has a broad range of applications across industry, engineering, and environmental science [4]. [5] investigated the effects of convective and radiative heat loss on CO_2 emission, O_2 depletion and thermal stability in a stockpile of combustible material at a steady state. Besides, the model equations for the nonlinear heat and mass transfer problem were derived and solved using Runge-Kutta-Fehlberg method with shooting technique. [6] proposed a nonlinear mathematical model to estimate CO_2 emission, O_2 depletion, and thermal decomposition in a stockpile of reactive material undergoing an exothermic chemical reaction inside a long cylindrical pipe, accounting for convective heat and mass transfer at its surface. Furthermore, [7] investigated the thermal decomposition of an electrically combustible visco-elastic material in a cylindrical stockpile, considering O_2 consumption. The nonlinear partial differential equations governing the problem were solved numerically using the bi-variate spectral collocation approach. [8] demonstrated that models based on chemical kinetics, heat- and mass transfer phenomena can yield accurate predictions of self-ignition temperatures. Despite mathematical modeling on climate change has been studied by some scholars, little has been explored in formulating mathematical model that simultaneously combines the transient (unsteady) effects of heat generation, oxygen emission and carbon dioxide emission, hence leading to the motivation for the current study.

2. Mathematical formulation

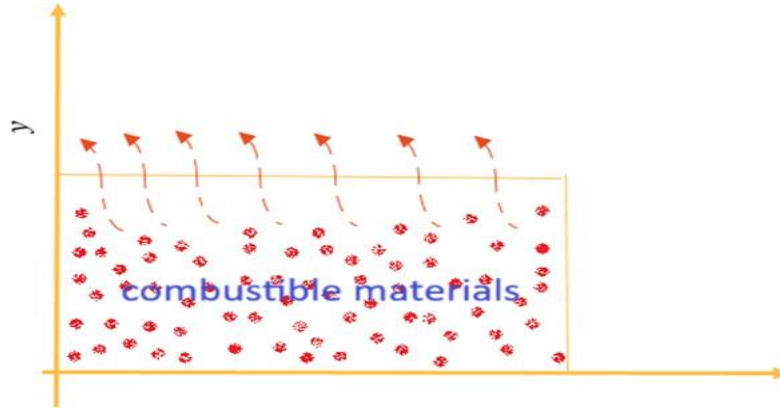
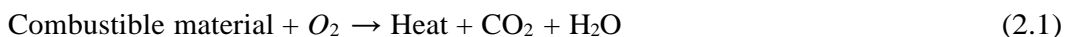


Figure 1: Schematic diagram

In formulating mathematical model, it was assumed that the combustible materials are stored on a rectangular slab and in it the oxidation reaction takes place. From the schematic diagram, the temperature dimensional T , Oxygen depletion O and the carbon dioxide C^* were derived for examination. It was further considered that the system is unsteady and heat transfer is governed by both conduction within the material and convective heat transfer.

The chemical reaction considered in the combustible materials in Fig. 1 is



Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

The reaction above shows that, for heat to occur, the oxygen gas must be consumed. This (inter alia) leads to heat and carbon dioxide gas. It is now becoming common to see fire occurring somewhere without someone causing it. The resulting model equations are:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_p} \frac{\partial^2 T}{\partial y^2} + \frac{QG}{\rho c_p} \left(\frac{KT}{vl} \right)^m O^n \frac{1}{\exp\left(\frac{E}{UT}\right)} \quad (2.2)$$

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_p} \frac{\partial^2 T}{\partial y^2} + \frac{QG}{\rho c_p} \left(\frac{KT}{vl} \right)^m O^n \frac{1}{\exp\left(\frac{E}{UT}\right)} \quad (2.3)$$

$$\frac{\partial O}{\partial t} = \beta \frac{\partial^2 O}{\partial y^2} - G \left(\frac{KT}{vl} \right)^m O^n \frac{1}{\exp\left(\frac{E}{UT}\right)} \quad (2.4)$$

$$\frac{\partial C}{\partial t} = \gamma \frac{\partial^2 C}{\partial y^2} + G \left(\frac{KT}{vl} \right)^m O^n \frac{1}{\exp\left(\frac{E}{UT}\right)} \quad (2.5)$$

subject to the conditions:

where t is the time, c_p is the specific heat at constant pressure, ρ is the density, k is the slabs conductivity, m is the numerical exponent, n is the order of exothermic reaction, Q is the exothermicity, G is the constant rate, K is the Boltzmann constant, l is the Planck number, v is the vibration frequency, E is the activation energy, U is the universal gas constant, D is the diffusivity of oxygen, γ is the diffusion of carbon dioxide in the slab T is the temperature, C the emission of carbon dioxide gas, O stands for the depletion oxygen, T_a , C_a , and O_a is the respectively ambient temperature, carbon dioxide and oxygen, a is half of the slabs width h_1 , h_2 and h_3 is respectively coefficient of heat transfer between the slab and its surroundings, coefficient of carbon dioxide transfer between the slab and its surroundings and coefficient of oxygen transfer between the slab and its surroundings.

3. Non-dimensionalization of the mode equations

The formulated model equations above are transformed into non-dimensional form using the following variables:

Substituting these non-dimensional values to the model equations 3.2 – 3.9 we get the following dimensionless equations. For convenience, the asterisks are dropped:

Annord Mwapinga

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \eta^2} + \Gamma (1 + \delta \theta)^m O^n \exp \left(\frac{\theta}{1 + \delta \theta} \right) \quad (3.2)$$

$$\frac{\partial O}{\partial \tau} = \alpha \frac{\partial^2 O}{\partial \eta^2} - \Gamma \Lambda_1 (1 + \delta \theta)^m O^n \exp \left(\frac{\theta}{1 + \delta \theta} \right) \quad (3.3)$$

$$\frac{\partial C}{\partial \tau} = \sigma \frac{\partial^2 C}{\partial \eta^2} + \Gamma \Lambda_2 (1 + \delta \theta)^m O^n \exp \left(\frac{\theta}{1 + \delta \theta} \right) \quad (3.4)$$

with boundary and initial conditions

$$\frac{\partial \theta}{\partial \tau}(0, \tau) = \frac{\partial C}{\partial \tau}(0, \tau) = \frac{\partial O}{\partial \tau}(0, \tau) = 0 \quad (3.5)$$

$$\theta(\eta, 0) = \theta_0, C(\eta, 0) = c_0, O(\eta, 0) = o_0 \quad (3.6)$$

$$\frac{\partial \theta}{\partial \eta}(1, \tau) = -b_1[\theta(1, \tau) - \theta_a] \quad (3.7)$$

$$\frac{\partial C}{\partial \eta}(1, \tau) = -b_2[C(1, \tau) - 1] \quad (3.8)$$

$$\frac{\partial O}{\partial \eta}(1, \tau) = -b_3[O(1, \tau) - 1] \quad (3.9)$$

where $\Gamma, \delta, \Lambda_1, \Lambda_2, \alpha, \sigma, b_1, b_2, b_3$ are respectively, Frank-Kamenetskii parameter, activation energy parameter, oxygen consumption rate parameter, carbon dioxide emission rate parameter, oxygen diffusivity parameter, carbon dioxide diffusivity parameter, the thermal Biot number, oxygen Biot number, and carbon dioxide Biot number.

4. Method of solution

The present study employs the finite difference method to solve the governing model equations, specifically utilizing the explicit scheme. This approach involves discretizing both the spatial and time domains. In the time discretization, a forward difference method was applied, while the spatial domain was discretized using central differences. This explicit scheme allowed the computation of the updated values at each grid point directly from the known values at the previous time step, eliminating the need for matrix inversion. Besides, the method is conditionally stable, and to ensure stability, the time step is chosen sufficiently small in relation to the spatial grid spacing. Additionally, the stability criterion, known as the Courant-Friedrichs-Lewy (CFL)

Condition $\left(0 < \frac{\Delta t}{(\Delta y)^2} \leq 0.5 \right)$ was observed in the implementation. Recently, several authors such as [9], [10], [11], [9]. [12] have employed such method to solve the differential equations.

The following schemes were considered:

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

Discretization of time:

$$\frac{\partial \theta}{\partial \tau} = \frac{\theta(i, k+1) - \theta(i, k)}{\Delta \tau}, \quad \frac{\partial C}{\partial \tau} = \frac{C(i, k+1) - C(i, k)}{\Delta \tau}, \quad \frac{\partial O}{\partial \tau} = \frac{O(i, k+1) - O(i, k)}{\Delta \tau} \quad (4.1)$$

Space discretization:

$$\frac{\partial^2 \theta}{\partial \eta^2} = \frac{\theta(i, k+1) - 2\theta(i, k) + \theta(i-1, k)}{(\Delta \eta)^2} \quad (4.2)$$

$$\frac{\partial^2 C}{\partial \eta^2} = \frac{C(i, k+1) - 2C(i, k) + C(i-1, k)}{(\Delta \eta)^2} \quad (4.3)$$

$$\frac{\partial^2 O}{\partial \eta^2} = \frac{O(i, k+1) - 2O(i, k) + O(i-1, k)}{(\Delta \eta)^2} \quad (4.4)$$

we further consider, $\theta = \theta(i, k)$, $C = C(i, k)$ and $O = O(i, k)$. Using the schemes, the model equations in discretized form become:

$$\theta(i, k+1) = \theta(i, k) + \Delta \tau \left(\frac{\theta(i, k+1) - 2\theta(i, k) + \theta(i-1, k)}{(\Delta \eta)^2} \right) + \Gamma(1 + \delta\theta(i, k))^m (O(i, k))^n \exp \left(\frac{\theta(i, k)}{1 + \delta(\theta(i, k))} \right) \quad (4.5)$$

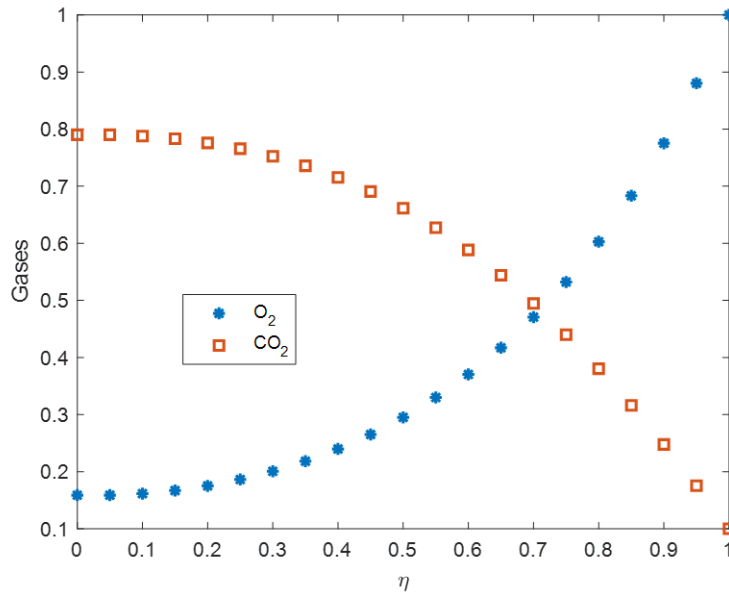
$$O(i, k+1) = O(i, k) + \Delta \tau \alpha \left(\frac{O(i, k+1) - 2O(i, k) + O(i-1, k)}{(\Delta \eta)^2} \right) - \Gamma \times \Lambda_1 (1 + \delta\theta(i, k))^m (O(i, k))^n \exp \left(\frac{\theta(i, k)}{1 + \delta(\theta(i, k))} \right) \quad (4.6)$$

$$C(i, k+1) = C(i, k) + \Delta \tau \sigma \left(\frac{C(i, k+1) - 2C(i, k) + C(i-1, k)}{(\Delta \eta)^2} \right) + \Gamma \times \Lambda_2 (1 + \delta\theta(i, k))^m (O(i, k))^n \exp \left(\frac{\theta(i, k)}{1 + \delta(\theta(i, k))} \right) \quad (4.7)$$

5. Results and discussion

Simulation of the results was done using MATLAB. Some flow parameters were varied to see their impact. Following [5], the following default values were used.

$m = 0.5, n = 1, \theta_a = 0.1, \alpha = 0.1, \sigma = 0.1, \Gamma = 0.1, \Lambda_1 = 0.1, \Lambda_2 = 1, \delta = 0.1$. Besides $\Delta \eta = 0.05$ and $\Delta \tau = 0.001$. the following graphs were simulated, temperature profiles, carbon dioxide profile and oxygen gas profile. the varied parameters were, Γ_1 ,



Γ_2 , δ , m , and n . Transient effects were also plotted accordingly.

Figure 2:

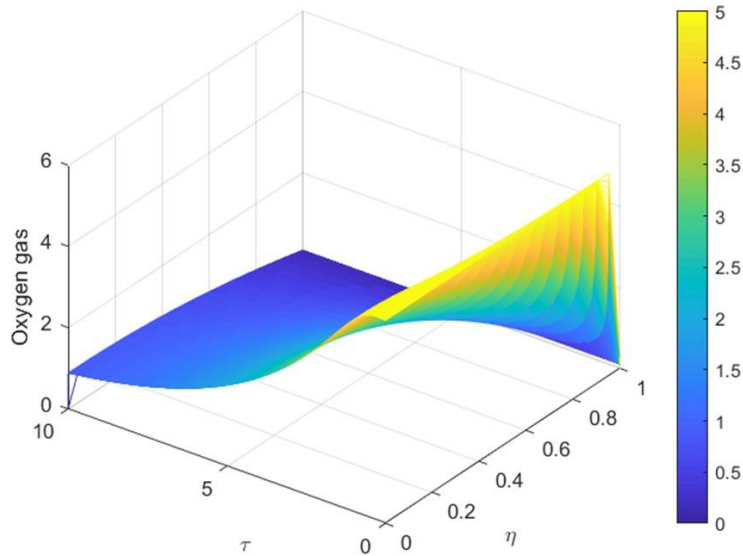


Figure 3: Transient Effects of Oxygen Concentration

Fig 2 shows the dynamics of both oxygen and carbon dioxide gases. From the graph, we observe that the oxygen gas declines while carbon dioxide is enhanced. The enhancement of the carbon dioxide gas increases the greenhouse gases in the atmosphere and eventually

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

increasing the temperature. Besides, oxygen gas is observed to decline because it is consumed to allow combustion. Fig 3 portrays the transient effects of the concentration of oxygen gas. The decrease of the amount of oxygen gas is a result of its consumption to allow combustion.

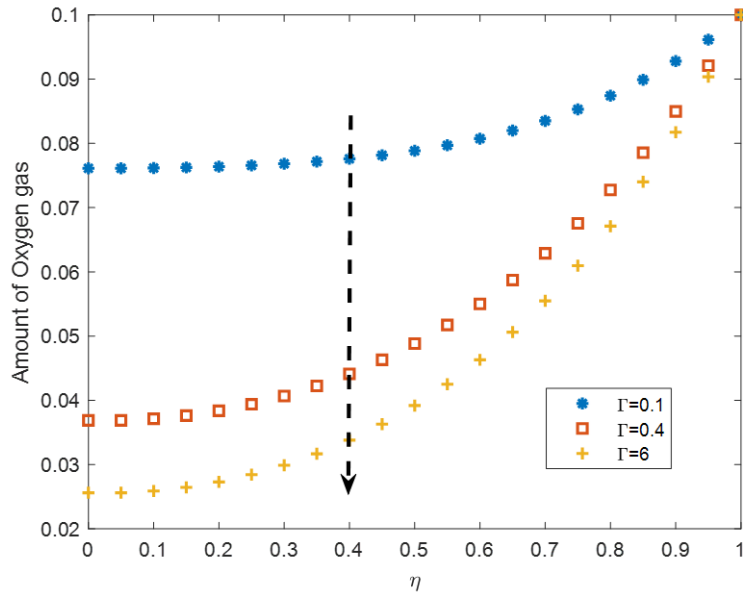


Figure 4: Effect of Frank-Kamenetskii parameter Γ on oxygen gas

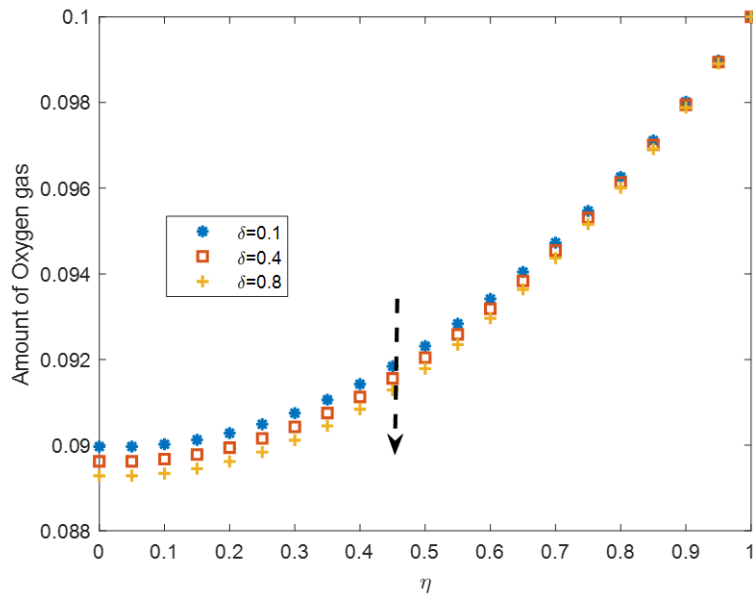


Figure 5: Effect of activation energy δ on oxygen gas

Annord Mwapinga

The effect of increasing Frank-Kamenetskii parameter Γ on oxygen is revealed on Fig. 4. Frank-Kamenetskii parameter dimensionless quantity helps us to analyze the heat generated by chemical reaction and heat dissipation (loss of heat to the surrounding). It is shown that increasing Frank-Kamenetskii parameter declines the amount of oxygen. Increasing Γ , implies that the heat resulted by chemical reaction is higher as compared to heat loss. This physically means that the chemical reaction is accelerated and hence more oxygen is consumed. It is worth noting that higher increase in parameter, potentially leads to thermal runaway, where the temperature rises uncontrollably and possibly causing a thermal explosion. The effect of activation energy on oxygen is shown on Fig. 5. Activation energy is the minimum amount of energy required for a chemical reaction to occur. It gradually slows down the consumption of oxygen gas. The gradual consumption is because it is the energy required to initiate a chemical reaction.

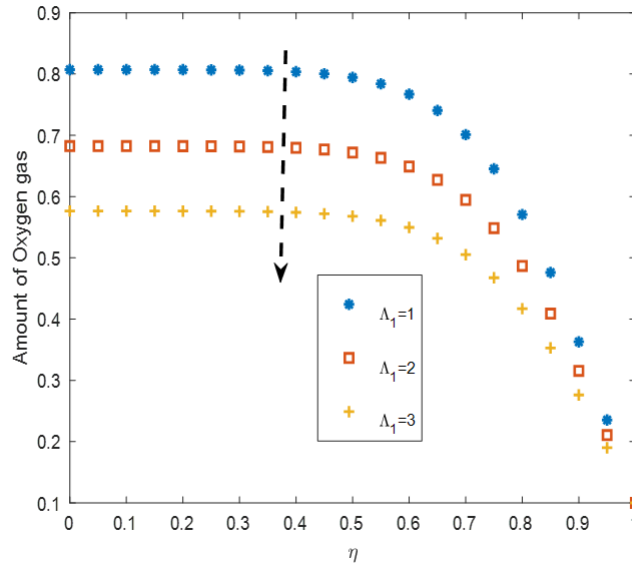


Figure 6: Effect of oxygen consumption parameter Λ_1 on O_2

Fig. 6 illustrates the influence of oxygen consumption parameter on amount of oxygen. The oxygen profile decreases with increase in Λ_1 . The same is observed when the diffusion parameter increases. See Fig. 7. Increased diffusion leads to higher oxidation to faster combustion. consequently, more oxygen is consumed.

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

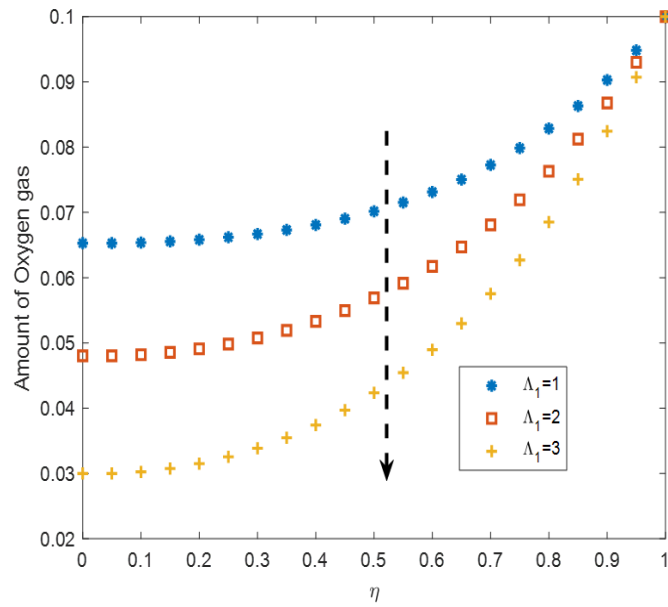


Figure 7: Effect of diffusion parameter on O_2

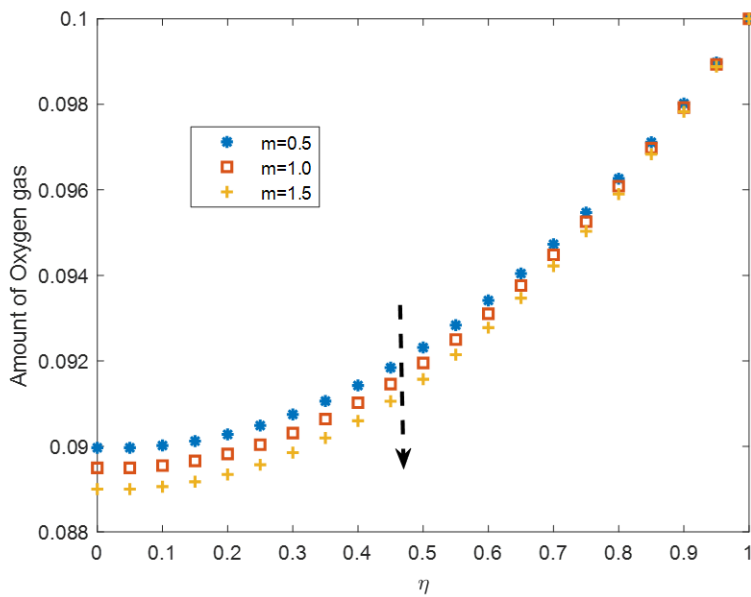


Figure 8: Effect of varying numerical exponent on O_2

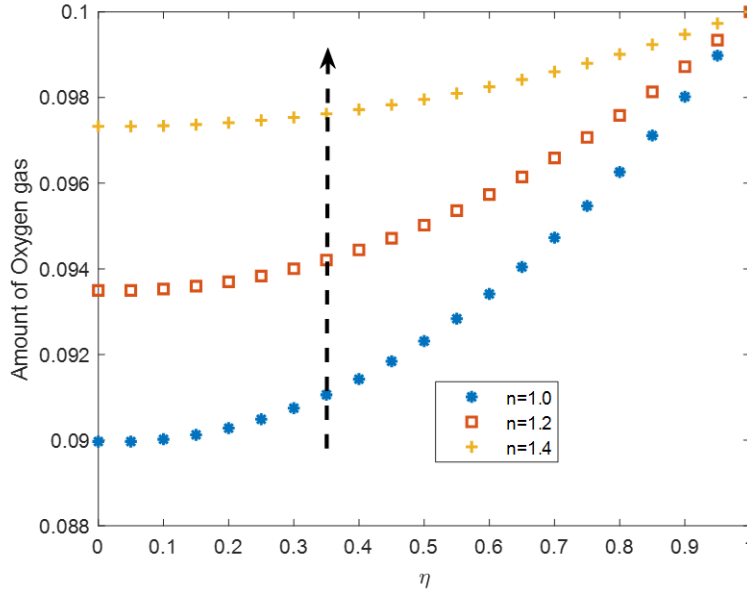


Figure 9: Effect of order of reaction on O₂

Figs. 8 and 9 show the effect of numerical exponent m and order of exothermic reaction n . It is revealed that oxygen consumption is enhanced more rapidly as the exponent increases. In an exothermic reaction, as the reaction rate increases, oxygen is consumed more quickly.

Here below the graphs for dynamics of the concentration of carbon dioxide are put in place. Chemically, carbon dioxide consists of one carbon atom covalently bonded to two oxygen atoms, giving it the chemical formula CO₂. Carbon dioxide gas is a significant greenhouse gas, meaning that it traps heat in the Earth’s atmosphere. When sunlight enters the atmosphere, it is absorbed by the Earth’s surface and re-radiated as infrared radiation.

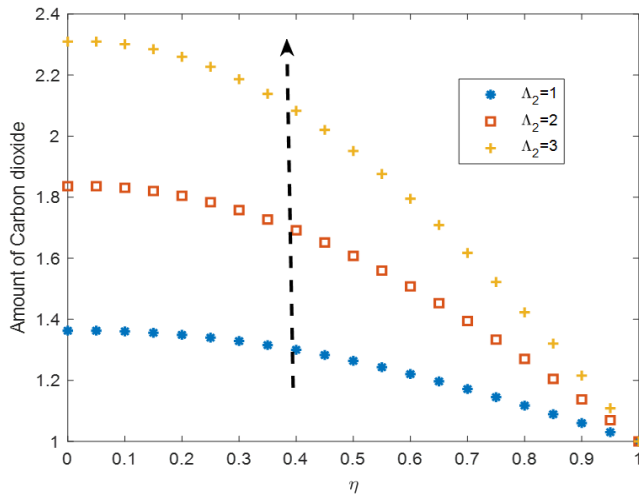


Figure 10: Effect of CO₂ emission rate on carbon dioxide

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

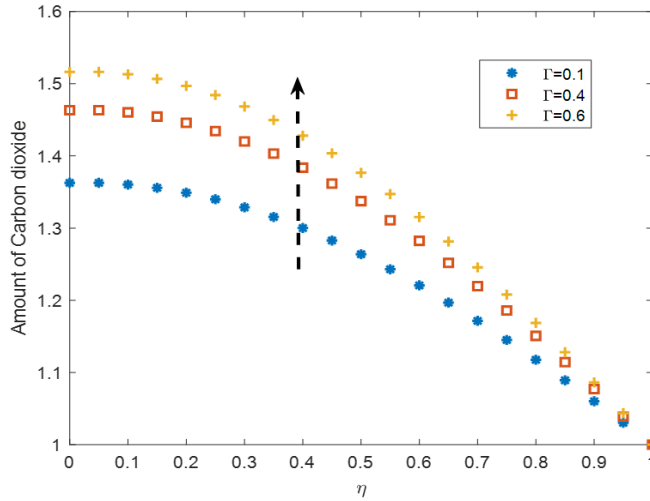


Figure 11: Effect of Frank-Kamenetskii parameter Γ on CO_2

The effect of emission rate on carbon dioxide concentration is shown on Fig. 10. The CO_2 increases with increase in Λ_2 . The same is observed (see Fig. 11) when Frank-Kamenetskii parameter Γ is increased. Physically, increasing Γ indicates that the heat generated by reaction is higher than its loss to the environment. Higher heat generation on the other hand, implies more oxygen is consumed and hence more CO_2 is released to the atmosphere as a product. Besides, Fig. 12 displays the mesh diagram (in three dimensions) of the carbon dioxide over time. It is clearly observed that over a time, the carbon dioxide is increased on the atmosphere. This has an impact to the climate change.

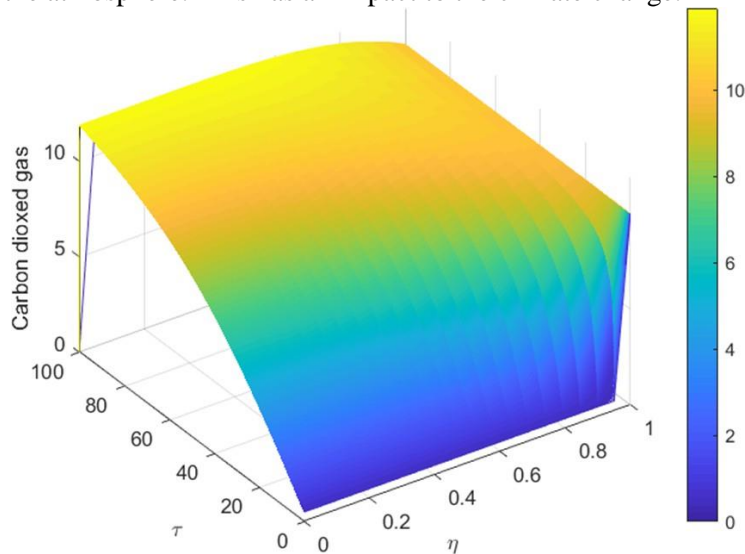


Figure 12: Transient effect of carbon dioxide gas

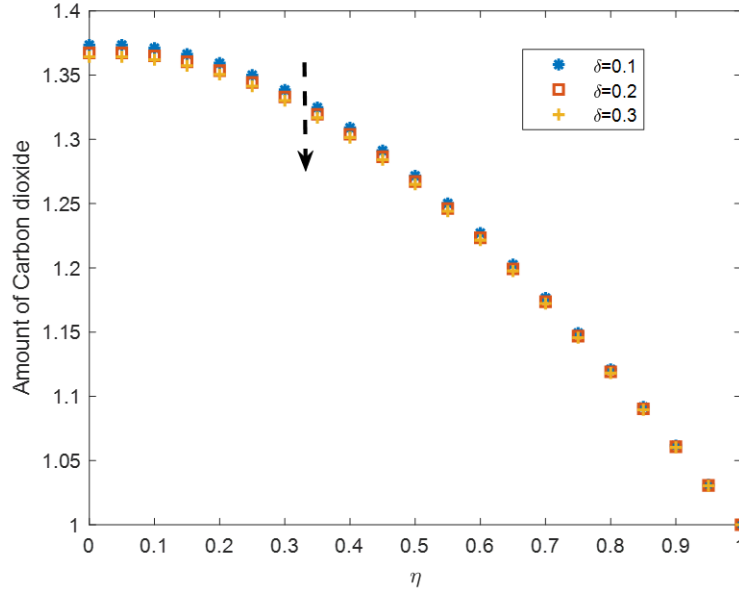


Figure 13: Effect of activation energy parameter δ on CO_2

Fig. 13 shows that the activation energy δ increases the CO_2 emission. Fundamentally, increasing the activation energy in stockpile combustion slows down the oxidation process which eventually delays the temperature rise, and lowers the production of CO_2 . That is higher activation energy makes the reaction little-bit less sensitive to temperature variations and slows down the exothermic reaction. To control our environment therefore, it is important we mold it in the manner that in any stockpile, the activation energy to be very high

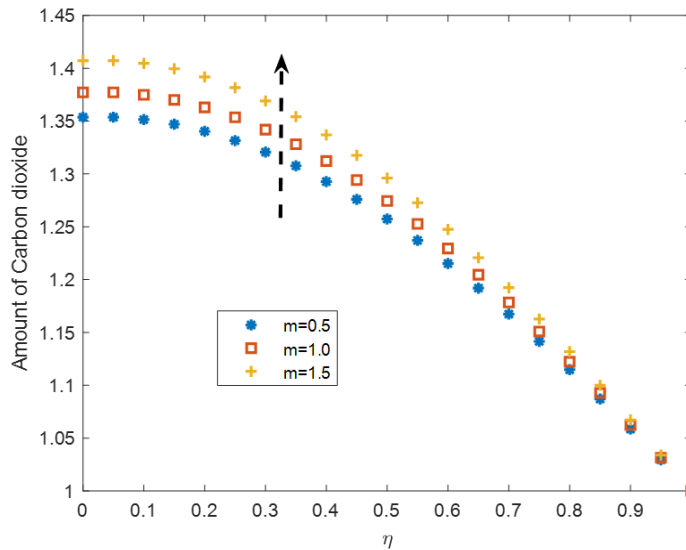


Figure 14: Effect of m on CO_2

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

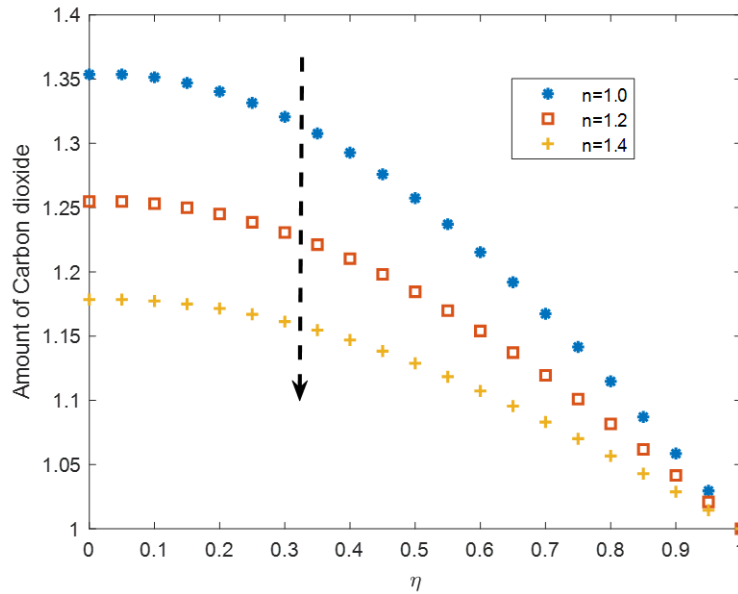


Figure 15: Effect of n on CO_2

The increase in m and n on the carbon dioxide shows different patterns. this is shown on Figs. 14 and 15. m is observed to enhance carbon dioxide while n declines the amount of carbon dioxide. It is worth noting that as the reaction rate increases (with higher order reactions), more oxygen is consumed and more carbon dioxide is produced per unit of time.

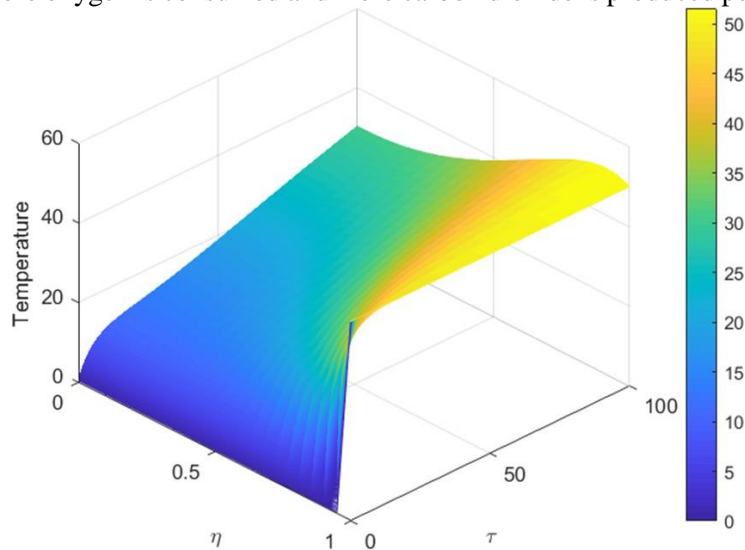


Figure 16: Transient effect of temperature

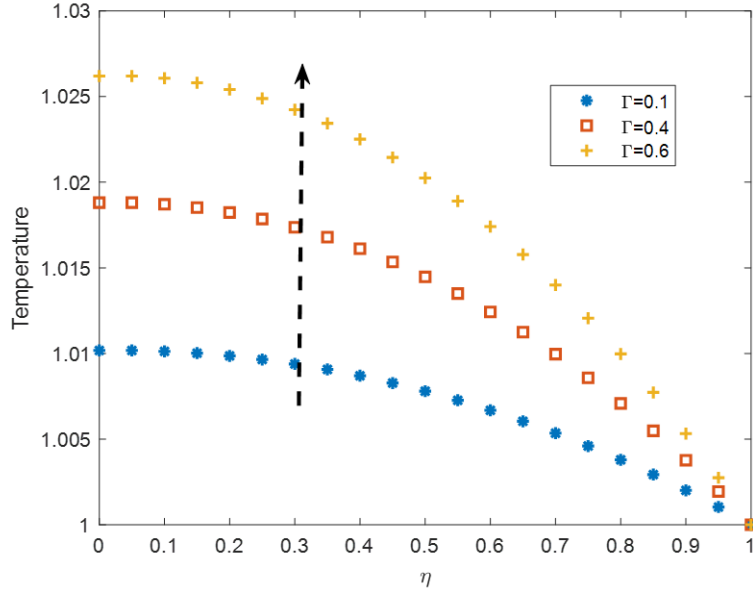


Figure 17: Effect of Frank-Kamenetskii parameter Γ on temperature

Fig. 16 shows the general transient effect of temperature over a time. The effect of Frank-Kamenetskii parameter Γ is displayed in Fig. 17. Increasing Γ means that the reaction increases and therefore the system has a greater possibility to experience thermal runaway. In other words, increasing Γ accelerates chemical reaction which leads to the increased temperature. Besides, increasing Γ on the other hand implies that the heat generated by reaction dominates heat lost to the surroundings, which results in a more rapid increase in temperature. In this regard therefore, for systems undergoing combustion or explosions, a higher Frank-Kamenetskii parameter can lead to more rapid ignition and potentially catastrophic runaway reactions if not controlled.

The effect of varying the activation energy on temperature is illustrated on Fig. 18. From the figure, we see that as δ increases, the temperature declines. This is due to the reason that, basically, $e^{E/UT}$ diminishes as E is enhanced. This means that at lower temperatures, the reaction slows down more significantly for higher activation energies. Besides, the pile will require more energy to start oxidation and hence making it difficult to maintain high temperatures unless sufficient heat is applied. The same behavior is revealed when oxygen consumption rate Λ_1 is varied.

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

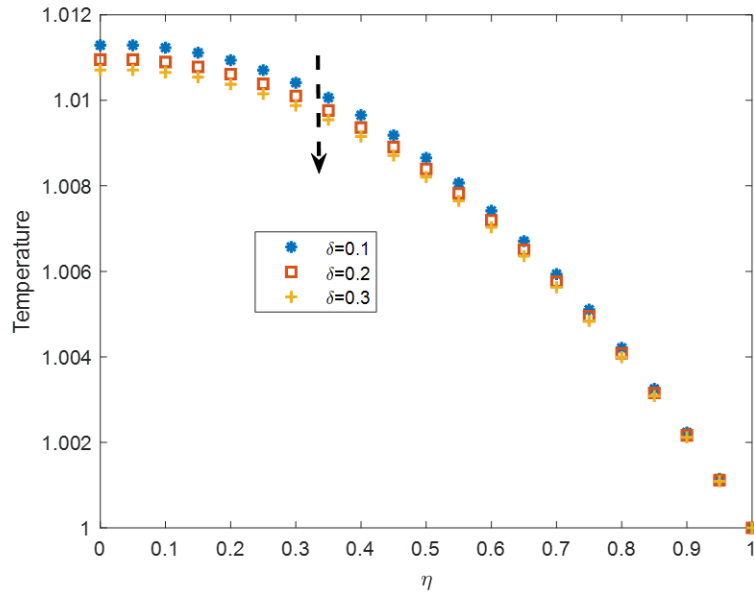


Figure 18: Effect of activation energy δ on temperature

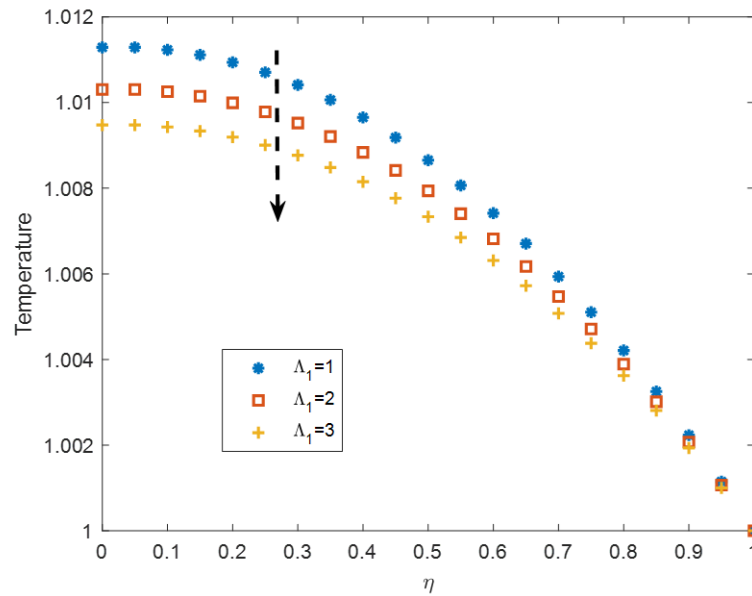


Figure 19: Effect of Λ_1 on temperature

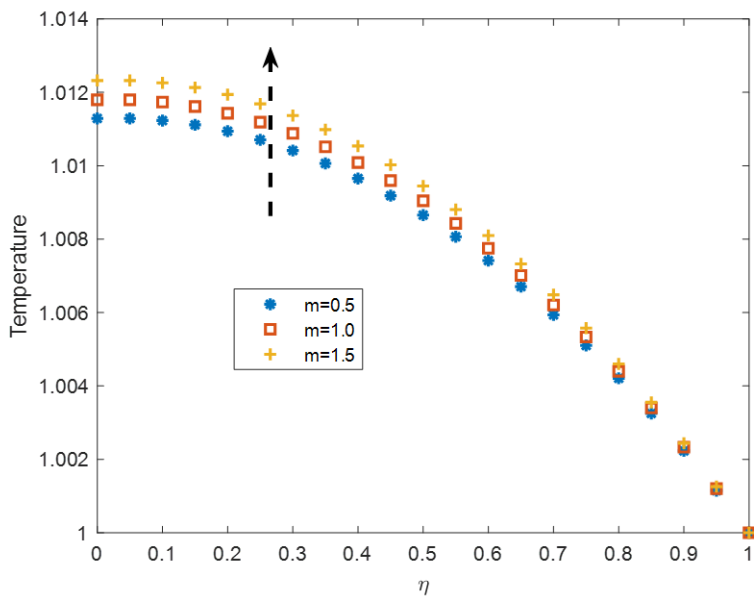


Figure 20: Effect of increasing numerical exponent on temperature

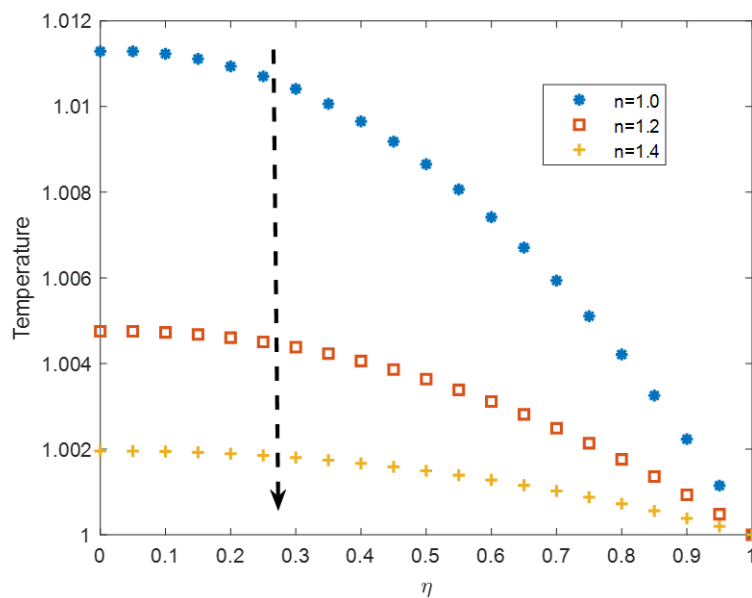


Figure 21: Effect of increasing order of reaction on temperature

The numerical exponent m and the order of reaction n show different patterns when are varied. The numerical exponent enhances temperature (see Fig 20) while the order of reaction reduces the temperature (see Fig 21).

Mathematical Modeling of Stockpile Combustion: Effects on Temperature, Oxygen Depletion and Carbon Dioxide Emission

6. Conclusion

The mathematical models that can analyze the unsteady dynamics of oxygen, carbon dioxide and temperature have been put in place. The effect of several parameters has been studied. This includes the Frank-Kamenetskii parameter and activation energy parameter. The study has found that the Frank-Kamenetskii parameter diminishes the amount of oxygen gas and enhances the carbon dioxide and temperature. On the other hand, the increase in activation energy is observed to reduce both, the amount of oxygen and temperature while it enhances the carbon dioxide gas emission. The oxygen consumption rate parameter Λ_1 is revealed to decline the amount of O_2 while the CO_2 emission rate parameter Λ_2 increases the carbon dioxide emission.

Acknowledgements. The author sincerely thanks the referee for their valuable suggestions, which have significantly improved the quality of the initial manuscript.

Author's Contributions: This work represents the sole contribution of the author.

Conflicts of interest. The author declares that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

REFERENCES

1. X.D. Chen, On the mathematical modelling of the transient process of spontaneous heating in a moist coal stockpile, *Combustion and Flame*, 90(2) (1992) 114–120.
2. A. Dueñas, G. Jiménez-Uzcátegui, and T. Bosker, The effects of climate change on wildlife biodiversity of the Galapagos islands, *Climate Change Ecology*, 2 (2001) 100026.
3. C. van Weelden, J.R. Towers, and T. Bosker, Impacts of climate change on cetacean distribution, habitat and migration, *Climate Change Ecology*, 1 (2021) 100009.
4. O. Makinde, T. Chinyoka, and R. Lebelo, Numerical investigation into CO_2 emission, O_2 depletion, and thermal decomposition in a reacting slab, *Mathematical Problems in Engineering*, 2011(1) (2011) 208426.
5. R.S. Lebelo and O.D. Makinde, Analysis of CO_2 emission, O_2 depletion and thermal stability in a convective and radiating reactive slab, *Global Journal of Pure and Applied Mathematics*, 13(2) (2017) 537–563.
6. T. Chinyoka and O. D. Makinde, Computational analysis of CO_2 emission, O_2 depletion and thermal decomposition in a cylindrical pipe filled with reactive materials, *Communications in Nonlinear Science and Numerical Simulation*, 18(9) (2013) 2448–2461.
7. A.T. Adeosun, S.O. Adesanya, R. S. Lebelo, and J. A. Gbadeyan, Mathematical investigation of a combustible visco-elastic material in a cylindrical stockpile with oxygen (O_2) consumption and induced electric field, *Numerical Heat Transfer, Part B: Fundamentals*, (2023) 1–21.
8. L. Schwarzer, P.A. Jensen, S. Wedel, P. Glarborg, O. Karlström, J. K. Holm, and K. Dam-Johansen, Self-heating and thermal runaway of biomass–lab-scale experiments and modeling for conditions resembling power plant mills, *Fuel*, 294 (2021) 120281
9. A. Mwapinga, Mathematical formulation and computation of the dynamics of blood flow, heat and mass transfer during MRI scanning, *Scientific Reports*, 14(1) (2024)

Annord Mwapinga

6364.

10. A. Mwapinga, Mathematical modeling of the physics of blood flow along a constricted artery during treatment of cancer using hyperthermia, *Computational Mathematics and its Applications*, (2024) 10–17.
11. A. Mwapinga, E. Mureithi, J. Makungu, and V.G. Masanja, Non-newtonian heat and mass transfer on mhd blood flow through a stenosed artery in the presence of body exercise and chemical reaction, 2020.
12. A. Mwapinga, E. Mureithi, J. Makungu, and V.G. Masanja, Mhd arterial blood flow and mass transfer under the presence of stenosis, body acceleration and chemical reaction: a case of magnetic therapy, 2020.