

Thermal Stability Analysis in a Two-Step Reactive Cylindrical Stockpile

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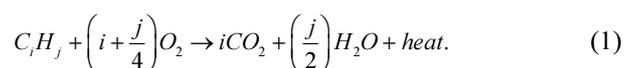
Abstract: Thermal stability analysis in a cylindrical stockpile of reactive material undergoing a two-step low-temperature oxidation reaction is studied in this article. The reactant consumption in this case is neglected and heat transfer with thermal stability are investigated by application of the energy equation. The complicated combustion process results with nonlinear interactions and hence the nonlinear partial differential equation governing the problem is tackled numerically using the semi-implicit Finite Difference Method (FDM). Kinetic parameters embedded on the governing partial differential equation, are varied to study the behavior of the temperature during the combustion process. The results are depicted graphically and adequately discussed, to bring an understanding of heat transfer and thermal stability during the combustion process. The study in this paper is relevant to multistep combustion process analogous to the fuel combustion in automobiles. The results, in general, show that thermal stability is more for sensitized chemical kinetics than for bimolecular type of kinetics.

Keywords: Thermal Stability, Heat Transfer, Two-Step Low-Temperature Oxidation Reaction, Cylindrical Pipe

Introduction

Spontaneous combustion due to a two-step low temperature oxidation reaction in a cylindrical stockpile of combustible material is investigated. Self-ignited fires in stockpiles of combustible materials are due to low-temperature oxidation reaction taking place between the carbon and the oxygen of the system. The study of runaway fires due to spontaneous combustion has attracted the interest of many researchers because some of veld fires that are hazardous to fauna and flora, are caused by self-ignition process (Nyamadzawo *et al.*, 2013). Spontaneous combustion takes place when the heat generated due to the low-temperature oxidation reaction (exothermic chemical reaction) in a stockpile of reactive material accumulates progressively and its release rate to the immediate surrounding is lesser compared to its generation rate (Lohrer *et al.*, 2005; Hensel *et al.*, 2004). The continued accumulation of heat in the system, makes the temperature to raise exponentially following the Arrhenius rate law (Taghikhani, 2011; Logan, 1982). Physical parameters or factors that affect self-ignition in stockpiles of combustible materials are, among others, the material particle size, the temperature of the environment,

the humidity of the material, the porosity and airflow rate of the stockpile (Lebelo, 2016; Schmidt *et al.*, 2003). The parameters listed above need experimentation to study their influence on the temperature gradients during combustion. In this case, theoretical approach to the study of heat transfer and the stability thereof during combustion process is done mathematically, with the use of computer programming. This approach requires good knowledge and understanding of the kinetic parameters embedded on the governing equation, which are properties of the combustible material and the reactant gas (Arisoy *et al.*, 2006). Many studies on heat transfer and thermal stability analysis in stockpiles of reactive materials were done by assuming a one-step, complete combustion, irreversible chemical reaction represented by Equation 1 (Lebelo, 2014; Legodi *et al.*, 2011; Lebelo and Makinde, 2015):



In this investigation, a two-step combustion process of reactive material, analogous to the combustion of fuel in automobile engines is considered. The first step of the

fuel combustion in an engine is incomplete and produces the toxic carbon monoxide. The second step helps to consume this toxic gas. The two-step chemical reaction taking place in autocatalytic converter used in the exhaust system is provided by the following equations (Makinde and Tshehla, 2013):



Thermal stability analysis of a two-step reactive slab was studied in (Makinde and Tshehla, 2013; Makinde *et al.*, 2013). The investigation in this article extends the work done to cylindrical domains and to the best knowledge of the author, no work, or very little, has been done in this regard, except for the mention of some applications of thermal stability investigation of reactive materials due to low-temperature oxidation reaction, which are, just to mention a few, in the improvement of the designing and the operations of engineering and industrial devices, the prevention of self-ignited fires, the packaging and the storage of reactive materials and the control of pollution (Lebelo *et al.*, 2016; Lebelo and Makinde, 2015) The combustion process is very complicated and results with many nonlinear interactions (Lebelo and Makinde, 2015), therefore, it is not possible to solve the governing partial differential equation exactly, but numerical methods are applied. In this case, the semi-implicit FDM embedded within the Maple software was used to solve the nonlinear differential equation. The article setup is as follows: the mathematical formulation is in section two and the numerical algorithm is given in section 3. Results and discussion are provided in section 4.

Mathematical Formulation

Unsteady State Combustion Process

Thermal stability investigation of a two-step low-temperature oxidation reaction in a stockpile of combustible material is considered in a cylindrical pipe whose thermal conductivity is constant. The material of the cylinder is assumed to undergo an n th order chemical reaction where the reactant consumption is neglected. The geometry of the problem is illustrated in Fig. 1.

The energy equation for the two-step low-temperature oxidation process, is expressed by the one dimensional nonlinear partial differential equation as (Makinde and Tshehla, 2013):

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + Q_1 A_1 C_1 \left(\frac{KT}{vl} \right)^m e^{-E_1/RT} + Q_2 A_2 C_2 \left(\frac{KT}{vl} \right)^m e^{-E_2/RT} - \varphi(T - T_b) \quad (4)$$

The initial condition is:

$$T(\bar{r}, 0) = T_0 \quad (5)$$

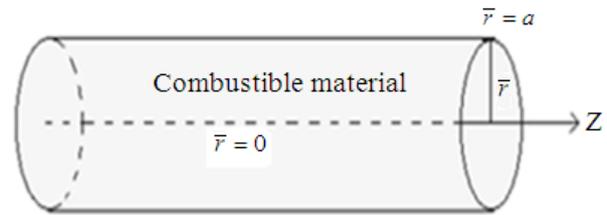


Fig. 1: Geometry of the problem

and the boundary conditions are:

$$\frac{\partial T}{\partial \bar{r}}(0, \bar{t}) = 0; T(a, \bar{t}) = T_b \quad (6)$$

In this case T is the cylinder's absolute temperature, T_0 is the initial temperature of the cylinder and T_b is the ambient temperature. p is the density, c_p is the specific heat at constant pressure, k is the thermal conductivity of the material, Q_1 , A_1 and C_1 are, respectively, the heat of reaction, the rate constant and the reactant concentration for the first step of the reaction and, Q_2 , A_2 and C_2 represent the heat of reaction, the rate constant and the reactant concentration, respectively, for the second step. In addition, K is the Boltzmann's constant, v is the vibration frequency, l is the 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 $m = 0.5$ is for the bimolecular kinetics and lastly, φ is the heat loss parameter (Lebelo, 2013; Lebelo and Makinde, 2015).

The following dimensionless parameters are introduced to Equation 4-6:

$$\theta = \frac{E_1(T - T_b)}{RT_b^2}, \theta_0 = \frac{E_1(T_0 - T_b)}{RT_b^2}, r = \frac{\bar{r}}{a}, \varepsilon = \frac{RT_b}{E_1}, \gamma = \frac{E_2}{E_1}, t = \frac{k\bar{t}}{\rho c_p a^2}, \delta = \frac{a^2 \varphi}{k}, \mu = \frac{Q_2 A_2 E_2}{Q_1 A_1 E_1} e^{(E_1 - E_2)/RT}, \lambda = \left(\frac{KT_b}{vl} \right)^m \frac{Q_1 A_1 E_1 a^2 C_1}{kRT_b^2} e^{-E_1/RT} \quad (7)$$

Equations 4-6 now have the following forms:

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r} + \lambda(1 + \varepsilon \theta)^m \left\{ e^{[\theta/(1 + \varepsilon \theta)]} + \mu e^{[\gamma \theta/(1 + \varepsilon \theta)]} \right\} - \delta \theta \quad (8)$$

The initial condition is:

$$\theta(r, 0) = \theta_0 \quad (9)$$

and boundary conditions are:

$$\frac{\partial \theta}{\partial r}(0, t) = 0; \theta(1, t) = 0 \quad (10)$$

where, θ is the dimensionless temperature, θ_0 is the dimensionless initial temperature, λ is the Frank-Kamenetskii parameter (reaction rate parameter), ε is the dimensionless activation energy parameter, r is the dimensionless radial distance, γ is the activation energy ratio parameter, μ is the two-step low-temperature oxidation parameter and δ is the dimensionless heat loss parameter.

Steady State Combustion Process

A steady state is attained at some time $t > 0$, where the rate of change of temperature with time is zero, that is $\frac{\partial \theta}{\partial t} = 0$, due to progressive thermal evolution of the reactive cylinder. The governing Equation 8 and its boundary equations become:

$$\frac{d^2 \theta}{dr^2} + \frac{1}{r} \frac{d\theta}{dr} + \lambda (1 + \varepsilon \theta)^m \left\{ e^{\left[\frac{\theta}{1+\varepsilon\theta}\right]} + \mu e^{\left[\frac{\gamma\theta}{1+\varepsilon\theta}\right]} \right\} - \delta \theta = 0 \quad (11)$$

$$\frac{d\theta}{dr}(0) = 0; \theta(1) = 0, \quad (12)$$

It is possible to obtain a solution series for the heat transfer rate at the surface of the cylinder and the Frank-Kamenetskii parameter λ , for some parameters values. The Nusselt Number (Nu), which is the dimensionless heat transfer rate at the surface of the cylinder, is given as (Lebelo, 2014; Legodi *et al.*, 2011; Lebelo and Makinde, 2015):

$$Nu = -\frac{d\theta}{dr}, \text{ at } r = 1 \quad (13)$$

Numerical Approach

To solve the nonlinear differential equation governing the problem, the semi-implicit finite difference scheme is applied. The implicit terms are taken at intermediate time level ($N + \zeta$) for $0 \leq \zeta \leq 1$. The intermediate time level $\zeta = 1$ was applied to enable the use of any larger time step. Numerical approximation of the governing partial differential equation is done by using the first and the second spatial derivatives with the second-order central differences. The modification of the equations corresponding to the first and last grid points helps to obtain the necessary boundary conditions. The discretization procedure to get the finite differences, is based on the linear Cartesian mesh and the uniform grid. The transformation of each component of the PDE is done as follows, (j represents position, N time and Δ_r mesh spacing).

The transformation of each component of the PDE is done as follows, (j represents position, N time and Δ_r mesh spacing):

$$\frac{\partial \theta}{\partial t} = \frac{\theta_j^{N+1} - \theta_j^N}{\Delta t} \quad (14)$$

$$\frac{\partial \theta}{\partial r} = \frac{1}{2\Delta r} \left[(\theta_{j+1}^{N+1} - \theta_{j-1}^{N+1}) + (\theta_{j+1}^N - \theta_{j-1}^N) \right] \quad (15)$$

and:

$$\frac{\partial^2 \theta}{\partial r^2} = \frac{1}{\Delta r^2} \left[(\zeta) (\theta_{j+1}^{N+1} - 2\theta_j^{N+1} + \theta_{j-1}^{N+1}) + (1-\zeta) (\theta_{j+1}^N - 2\theta_j^N + \theta_{j-1}^N) \right] \quad (16)$$

Therefore, the semi-implicit FDM for the governing equation is expressed as:

$$\frac{\theta_j^{N+1} - \theta_j^N}{\Delta t} = \frac{\partial^2}{\partial r^2} \theta^{N+\zeta} + \frac{1}{r} \frac{\partial}{\partial r} \theta^N + \lambda \left\{ (1 + \varepsilon \theta)^m e^{\left[\frac{\theta}{1+\varepsilon\theta}\right]} + \mu e^{\left[\frac{\gamma\theta}{1+\varepsilon\theta}\right]} \right\}^N - \delta \theta^N \quad (17)$$

The unknown time terms ($N + 1$) are put on the left and on the right the known time terms (N) are placed, to give the following equation:

$$\begin{aligned} & -\zeta \tau \theta_{j+1}^{N+1} + (1 + 2\zeta \tau) \theta_j^{N+1} - \zeta \tau \theta_{j-1}^{N+1} \\ & = -\tau (1 - \zeta) \theta_{j+1}^N + [1 - 2\tau (1 - \zeta) - \delta] \theta_j^N - \\ & \tau (1 - \zeta) \theta_{j-1}^N + \frac{1}{2r_j} \tau (\theta_{j+1}^N - \theta_{j-1}^N) + \\ & \lambda \Delta t \left\{ (1 + \varepsilon \theta)^m e^{\left[\frac{\theta}{1+\varepsilon\theta}\right]} + \mu e^{\left[\frac{\gamma\theta}{1+\varepsilon\theta}\right]} \right\}^N. \end{aligned} \quad (18)$$

Here, $\tau = \frac{\Delta t}{\Delta r^2}$ from Equation 18, a tri-diagonal system is formed and Maple software was used to give the graphical solutions.

Results and Discussion

The effects of thermo-physical parameters on the temperature gradient during combustion process, are depicted graphically and analyzed appropriately in this section. Heat transfer analysis during the steady state is done under subsection 4.1. Subsection 4.2 deals with heat transfer rate analysis for some set of parameters values. The third part, subsection 4.3, deals mainly with thermal stability analysis for a given set of parameters values. Unless otherwise stated, the following parameters assigned arbitrary values were used for the investigation:

$$m = 0.5, \mu = 0.1, \gamma = 0.1, \delta = 1, \lambda = 0.1, \varepsilon = 0.1, t = 10.$$

Steady State Transient Heat Analysis

The steady state is attained when the system temperature is independent of time. This is illustrated in Fig. 2 and 3, which show the temperature behavior with increasing time. It is observed that, as the time reaches higher values, the steady state is attained when the temperature profiles do no more increase with time. It is also observed that the temperature profiles are higher at the center of the cylinder and reduce to zero toward the surface thereof. This is due to progressive heat loss to the surrounding environment at the surface of the cylinder.

Kinetic Parameters' Effects on Temperature

Here, the effects of selected parameters on the temperature of the system are studied. The study is done by varying one parameter while keeping others constant and observing the temperature profile patterns to get an understanding of the heat transfer process. Figure 4 to 9 illustrate the effects of varied kinetic parameters on the temperature during the combustion process. A combined increase in the parameters λ (reaction rate), ε (activation energy), μ (two-step low-temperature oxidation), γ (activation energy ratio) and m (kinetic reaction type index), show a corresponding increase in the temperature profiles. Fig. 4 shows that an increase in the reaction rate facilitates the low-temperature oxidation process, which generates more heat into the system to raise its temperature. The increase in the activation energy of the system also encourages more generation of heat during combustion process, as indicated by Fig. 5. An increase in μ , depicted by Fig. 6, allows more of the reactant into the system to enhance the low-temperature oxidation reaction process. This process increases the rate of heat generation within the combusting material of the cylinder, to raise the system's temperature. The same scenario is illustrated in Fig. 7, where higher values of γ also encourage the taking place of the low-temperature oxidation process. It is interesting to note that the low-temperature oxidation reaction is faster in bimolecular type of chemical reaction ($m = 0.5$), compared to the Arrhenius type ($m = 0$) and that in the sensitized kinetics ($m = -2$), spontaneous ignition is slow, as depicted in Fig. 8. A different scenario is portrait in Fig. 9, which shows that an increase in δ (heat loss parameter), lowers the temperature of the system. This is due to progressive heat loss to the ambient at the surface of the cylinder. This parameter retards the accumulation of heat generated due to low-temperature oxidation reaction in the reactive cylinder, by lowering the temperature of the system. The parameter is also important to facilitate attainment of thermal stability of the system during the combustion process. Thermal stability is discussed in detail in the next subsection.

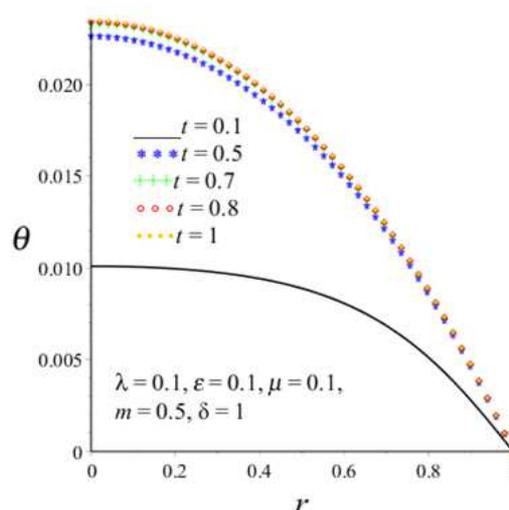


Fig. 2: 2-D steady state profile

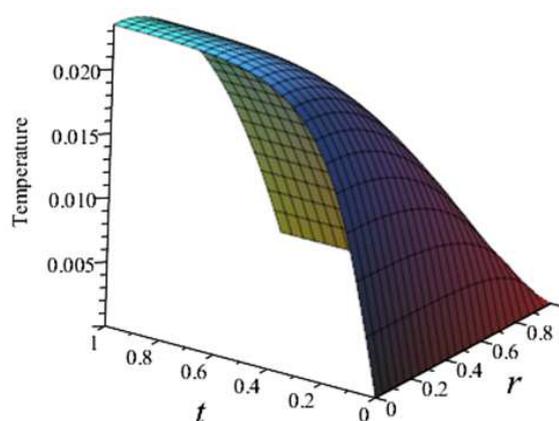


Fig. 3: 3-D steady state profile

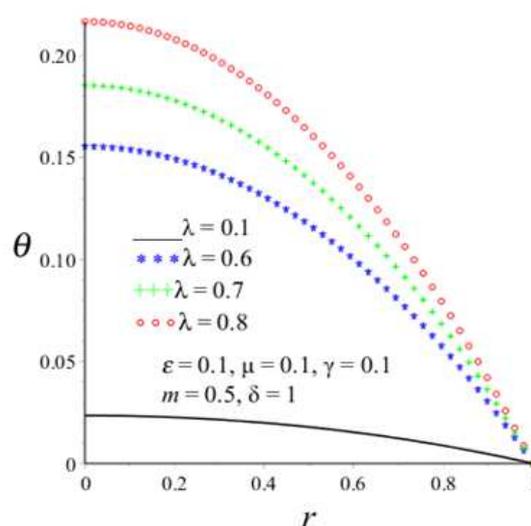


Fig. 4: λ effect on temperature

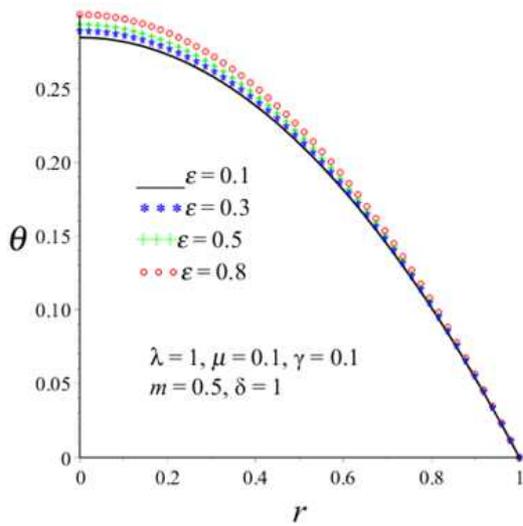


Fig. 5: ϵ effect on temperature

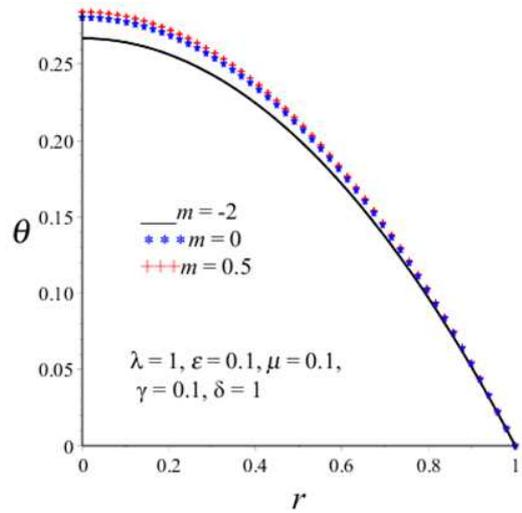


Fig. 8: m effect on temperature

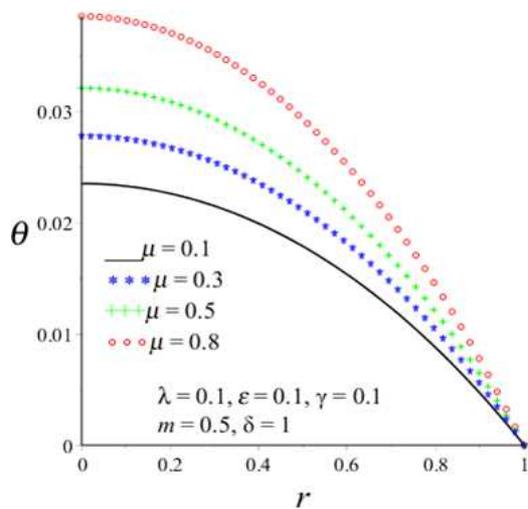


Fig. 6: μ effect on temperature

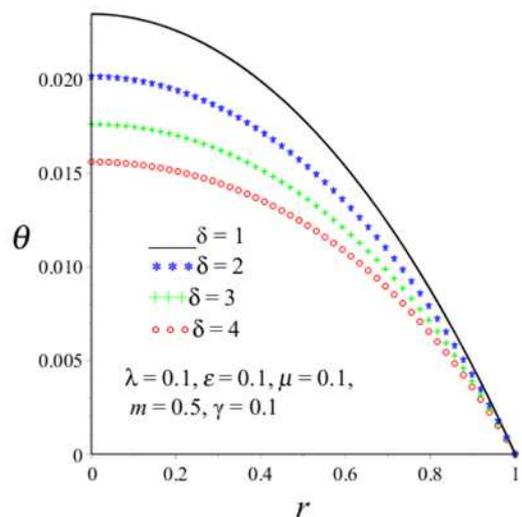


Fig. 9: δ effect on temperature

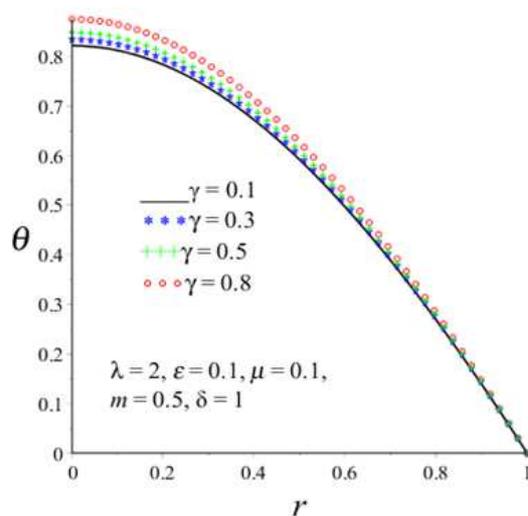


Fig. 7: γ effect on temperature

Thermal Stability Analysis

In this subsection, thermal stability analysis during combustion process is considered. For a combusting system to attain thermal stability, it is important to know criticality values which should not be exceeded to avoid the system from explosions. Criticality values (λ_c), are usually obtained from bifurcation diagrams, but in this case, the values are obtained from plotting the Nusselt Number (Nu) against the reaction rate parameter, also called the Frank-Kamenetskii parameter (λ), for some parameter values. Figure 10 to 14 depict criticality values in graphical form. The shortest graph represents the lowest value of the criticality value (λ_c), for example, the parameter $m = 0.5$ gives $\lambda_c = 2.4080$ which is the shortest graph in Fig. 10 and it demonstrates thermal instability for bimolecular kinetics.

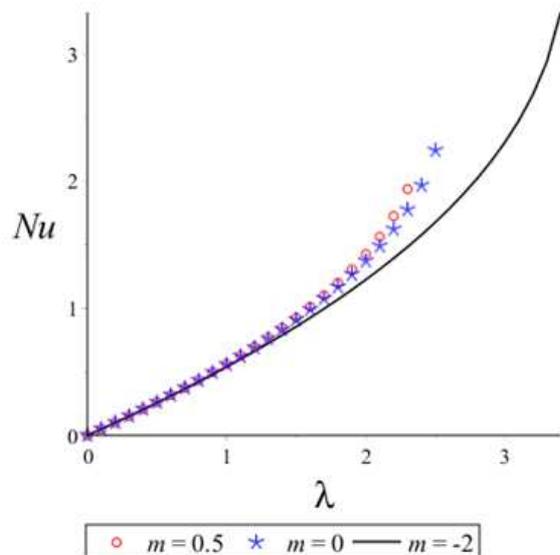


Fig. 10: m effect on thermal stability

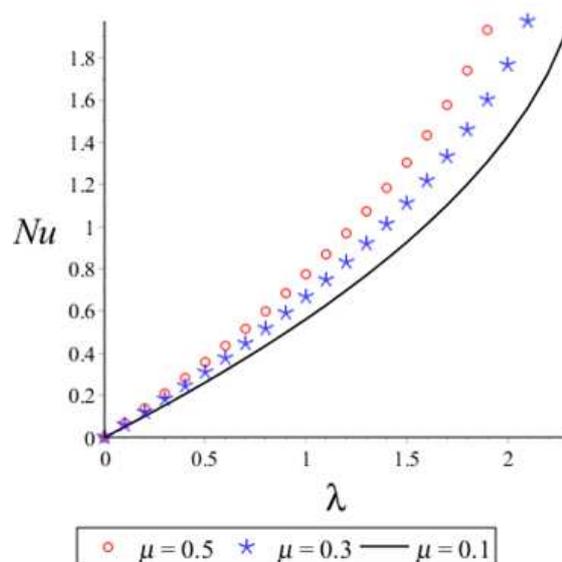


Fig. 12: μ effect on thermal stability

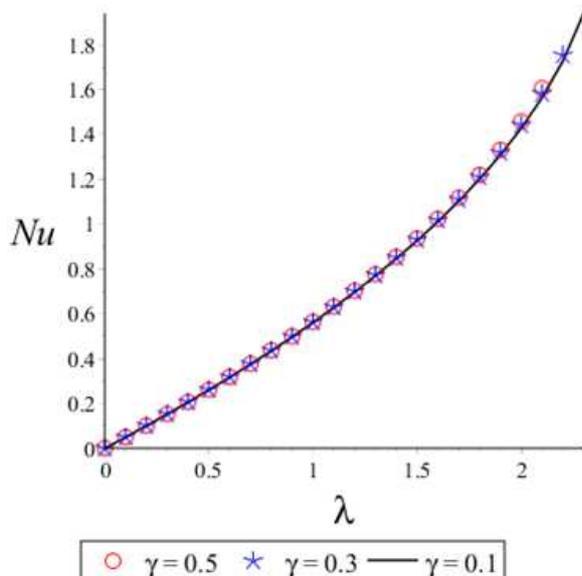


Fig. 11: γ effect on thermal stability

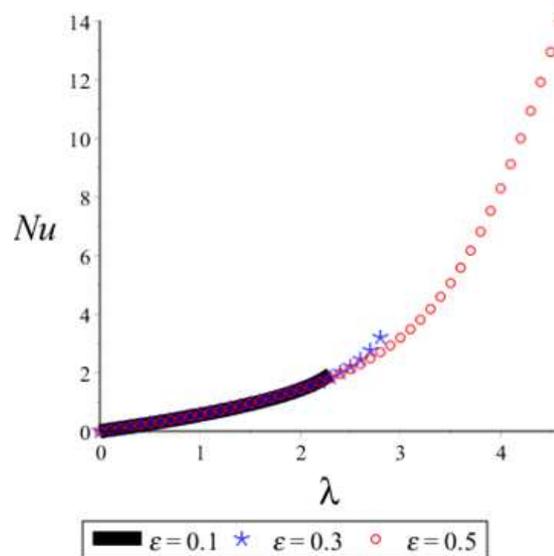


Fig. 13: ε effect on thermal stability

In the same Fig. 10, it is observed that $m = -2$ yields $\lambda_c = 3.4514$ to give the longest graph, illustrating the delay of the combustion explosion point by obtaining the largest criticality value, which represents thermal stability attainment. The criticality values (λ_c) and the Nusselt number values obtained for parameters m , ε , μ , γ and δ , are provided in Table 1.

We observe from Fig. 10 to 12 that a combined increase in parameters m , μ and γ , results with a decline in λ_c values. It is important to note that thermal stability is highest in sensitized kinetics, followed by Arrhenius kinetics and that it is low in bimolecular kinetics.

It is better to keep the values of μ and γ very low to attain thermal stability of the system. A combined increase in the parameters ε and δ , shows a corresponding increase in λ_c values, as depicted in Fig. 13 and 14. Thermal stability is achieved by keeping higher values of these parameters. Keeping the activation energy (ε) level very high, slows down the low-temperature oxidation reaction and therefore thermal stability is maintained. The higher values of the heat loss parameter (δ), imply increased heat loss rate at the surface of the cylinder to enhance the cooling down of the system, hence the achievement of thermal stability.

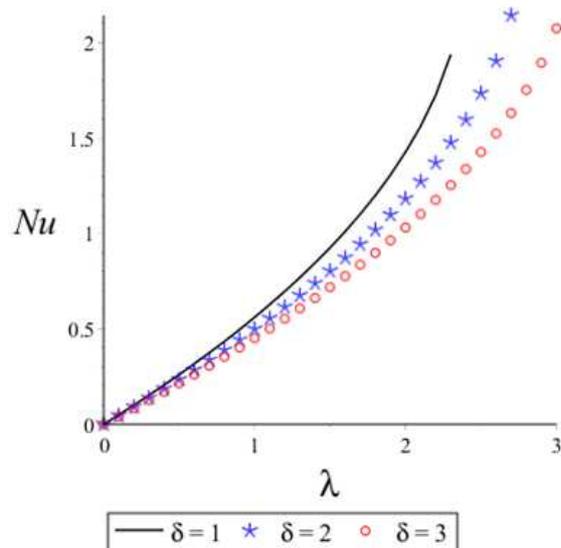


Fig. 14: δ effect on thermal stability

Table 1: Numerical values for Nu and λ_c obtained from effects of thermo-physical parameters on thermal stability, calculated using Maple software

m	μ	γ	ϵ	δ	Nu	λ_c
-2	0.1	0.1	0.1	1	3.88387	3.4514
0	0.1	0.1	0.1	1	2.67268	2.5593
0.5	0.1	0.1	0.1	1	2.48885	2.4080
0.5	0.3	0.1	0.1	1	2.67329	2.2469
0.5	0.5	0.1	0.1	1	2.83845	2.1128
0.5	0.1	0.3	0.1	1	2.48529	2.3879
0.5	0.1	0.5	0.1	1	2.47350	2.3631
0.5	0.1	0.1	0.3	1	4.98381	2.9241
0.5	0.1	0.1	0.5	1	16.05800	4.7794
0.5	0.1	0.1	0.1	2	2.53317	2.7644
0.5	0.1	0.1	0.1	3	2.58136	3.1212

Conclusion

The investigation in this article considered a combustion process which involves a two-step low-temperature oxidation reaction. The study was modeled in a cylindrical domain whose material is assumed to be of constant thermal conductivity. The first part of the study considered heat transfer analysis from the behavior of temperature due to effects of variation of selected kinetic parameters. The following parameters, m , ϵ , μ , γ and λ , were found to enhance the low-temperature oxidation reaction which generates heat to cause temperature raise of the system. The only parameter which facilitates the lowering of the temperature during the combustion process, was found to be δ , which does so by allowing heat loss at the cylinder's surface. The second part of the investigation dealt with analysis of thermal stability at steady state of the combustion process.

Criticality values, which are values not be exceeded to avoid explosions or self-ignition from taking place during combustion, were determined for selected kinetic parameters. It was found that thermal stability is achieved by lowering the values of the parameters m , μ and γ . A different scenario was observed from the parameters ϵ and δ , which help to maintain thermal stability by keeping their values very high. This investigation was done theoretically and the benefit thereof is that the understanding of the process of combustion due to low-temperature oxidation reaction, is acquired in a quicker and a cheaper way without the hazards that may be encountered with experiments. This study can be extended to combustible materials with temperature dependent thermal conductivity and, also to spherical domains.

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Author's Contributions

R.S. Lebelo: Problem conceptualization, and writing.
R.K. Mahlobo: Grammar correction and editing.
K.C. Moloi: Grammar correction and final editing.

Conflict of Interest

The author hereby declares that there is no conflict of interest on the publication of this manuscript.

References

- Arisoy, A., B.B. Beamish and E. Cetegen, 2006. Modelling combustion of coal. *Turk. J. Eng. Environ. Sci.*, 30: 193-201.
- Hensel, W., U. Krause and U. Löffler, 2004. Self-Ignition of Materials (Including Dust). In: *Handbook of Explosion Prevention and Protection*, Hartwig, M. and H. Steen, (Eds.), Weinheim: Wiley-VCH, pp: 227-270.
- Lebelo, R.S. and O.D. Makinde, 2015. Modelling the impact of radiative heat loss on CO₂ Emission, O₂ depletion and thermal stability in a reactive slab. *IJST, Trans. Mechan. Eng.*, 39: 351-365.
- Lebelo, R.S. and O.D. Makinde, 2015. Numerical investigation of CO₂ emission and thermal stability of a convective and radiative stockpile of reactive material in a cylindrical pipe. *Adv. Mech. Eng.*, 7: 1-11.
- Lebelo, R.S., 2016. Thermal stability investigation in a reactive sphere of combustible material. *Adv. Math. Phys.*, 2016: 1-6.

- Lebelo, R.S., 2014. Numerical investigation of CO₂ emission and thermal stability of a convective and radiative stockpile of reactive material in a cylindrical pipe of variable thermal conductivity. AIP Conf. Proc. 1621: 60-68.
- Lebelo, R.S., O.D. Makinde and K.O. Okosun, 2016. Numerical investigation of thermal stability in a reactive sphere of variable thermal conductivity. Global J. Pure Applied Math., 12: 4335-4347.
- Legodi, A.M.K. and O.D. Makinde, 2011. A numerical study of steady state exothermic reaction in a slab with convective boundary conditions. Int. J. Phys. Sci., 6: 2541-2549.
- Logan, S.R., 1982. The origin and status of the Arrhenius equation. J. Che. Ed., 59: 279-281.
- Lohrer, C., U. Krause and J. Steinbach, 2005. Self-ignition of combustible bulk materials under various ambient conditions. Process Safety Environ. Protection, 83: 145-150. DOI: 10.1205/psep.04234
- Makinde, O.D. and M.S. Tshehla, 2013. Analysis of thermal stability in a convecting and radiating two-step reactive slab. Adv. Mech. Eng., 2013: 1-9.
- Makinde, O.S., K.S. Adegbe and O. A. Fasoranbaku, 2013. Mathematical modelling of two-step exothermic reactions with and without reactants consumption. FUTA J. Res. Sci., 1: 44-53.
- Nyamadzawo, G., W. Gwenzi, A. Kanda1, A. Kundhlande and C. Masona, 2013. Understanding the causes, socio-economic and environmental impacts and management of veld fires in tropical Zimbabwe. Fire Sci. Rev., 2: 1-13.
- Schmidt, M., C. Lohrer and U. Krause, 2003. Self-ignition of dust at reduced volume fractions of ambient oxygen. J. Loss Prev. Proc. Ind., 16: 141-147.
- Taghikhani, M.A., 2011. Power transformer insulation lifetime estimation methods. Int. J. Energy Eng., 1: 9-11.