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Numerical Investigation of Thermal Stability in Media of Different Physical Geometries

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Abstract: Spontaneous combustion in stockpiles of combustible materials is due to exothermic chemical reaction taking place within the system, where the trapped oxygen reacts automatically with the material containing carbon or hydrocarbons. The chemical reaction results with heat as one of the products. Should the rate of heat production exceed that of heat release to the ambient, the system's temperature increases rapidly and may lead to thermal runaway that ultimately causes self-ignition. In this study, effects of kinetic parameters such as activation energy and rate of reaction on the temperature of the system are investigated. These parameters are embedded on the differential equation governing the problem. The combustion reaction results with complicated reaction mechanism that is nonlinear and as a result the nonlinear differential equation is tackled using numerical methods. Runge-Kutta-Fehlberg (RKF45) method coupled with shooting technique is used to solve the equation with the help of Maple Software.

Key words: Thermal stability, reactive slab, reactive cylinder, reactive sphere, Runge-kutta Fehlberg method, embedded

INTRODUCTION

Thermal stability in stockpiles of combustible materials has been investigated for physical parameters such as material particle size, volume-to-surface ratio, porosity, thermal conductivity, density and heat capacity, just to mention a few (Lohrer *et al*., 2005; Hensel *et al*., 2004). The interest in this investigation is due to self-ignited fires in stockpiles of combustible materials such as coal, hay, wood and wool, just to mention a few, that are hazardous to living species (Lebelo and Makinde, 2015a, b; Makinde, 2012a, b).

In this study, we investigate kinetic parameter's effects such as activation energy and rate of reaction parameters on the temperature behavior of the system to understand thermal stability pattern is media of different physical geometries. Several researchers like Hamza *et al*. (2011) and Lebelo (2014, 2015) investigated thermal stability in a reactive slab with or without reactant consumption. The investigation of thermal stability in a long cylindrical pipe of reactive material was done by Makinde (2005) and Lebelo (2015).

In this investigation, we include spherical domain and compare thermal stability in a reactive slab, reactive cylinder and reactive sphere. The significance of thermal stability investigation is to help with understanding of improvement of the design and operation of a number of industrial and engineering appliances (Makinde and Tshehla, 2013; Bebernes and Eberly, 1989). Most of industrial products' quality is affected by internal heat generation, due to exothermic chemical reaction, after casting, coating, molding or lamination. This is indicated by discoloring and even deforming out of shape by some industrial products. A common example of applicability of thermal stability is in preventing the damage caused by self-ignition in stockpiles of hay, wool or wood (Lebelo and Makinde, 2015, Lacey and Wake, 1982).

The exothermic chemical reaction taking place within a stockpile of combustible material results with a process that is very complicated. The complicated process is modelled mathematically and simplified by assuming a one dimensional nonlinear differential equation that governs the problem. RKF4 coupled with shooting technique is used to tackle the nonlinear differential equation numerically with the help of Maple software. The graphical solutions obtained for various embedded kinetic parameters on temperature behavior of the system are used to compare thermal stability in a slab, cylinder and sphere in order to achieve the objective of this study.

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MATERIALS AND METHODS

Mathematical formulation: We consider a stockpile of combustible material that is modelled in three different media of different physical geometries. The three media are: a rectangular slab, a long cylindrical pipe and a spherical domain and a constant thermal conductivity is assumed. Each physical geometry is assumed to undergo nth order exothermic chemical reaction with no reactant consumption accompanied by possibility of heat loss to the ambient (Fig. 1).

A steady state of an exothermic chemical reaction is considered and the complicated chemistry involved in this process is simplified by assuming a one-step finite rate irreversible Arrhenius kinetics. The one dimensional nonlinear ordinary differential equation that governs the problem is expressed generally as:

$$\frac{k}{\bar{\tau}^{M}}\frac{d}{d\bar{\tau}}\left(\bar{\tau}^{M}\frac{dT}{d\tau}\right)+QAC\left(\frac{KT}{vl}\right)^{m} e^{-E}/RT-\varphi(T-T_b)=0 \quad (1)$$

The boundary conditions are:

$$\frac{dT}{d\bar{\tau}}(0)=0;\ T(a)=T_b \quad (2)$$

In this case M = 0 is for the slab, M = 1 is for the cylinder and M = 2 is for the sphere. The symbol $\bar{\tau}$ represents $\bar{y}$ (slab rectangular distance) or $\bar{r}$ (radial distance of the cylinder or the sphere). T is the medium's absolute temperature T_0 is the initial temperature of the medium and T_b is the ambient temperature. K is the thermal conductivity of the material, Q is the heat of reaction, A is the rate constant and C is the reactant concentration. We have K as the Boltzmann's constant,v as the vibration frequency, 1 as the Planck's number, E as the activation energy, R as the universal gas number and m as the numerical exponent that takes the following values, -2 for sensitized, 0 for Arrhenius and 1/2 for bimolecular kinetics. Lastly, φ is the heat loss parameter (3, 6, 8, 9). The following dimensionless parameters are introduced to Eq. 1 and 2:

$$\theta=\frac{E(T-T_b)}{RT_b^2},\ \theta_0=\frac{E\,(T_0-T_b)}{RT_b^2},\ \tau=\frac{\bar{\tau}}{a},\ \varepsilon=\frac{RT_b}{E},$$
$$\delta=\frac{a^2\varphi}{k},\ \lambda=\left(\frac{KT_b}{vl}\right)^{m}\frac{QAEa^2C}{kRT_b^2}\exp\left(-\frac{E}{RT_b}\right) \quad (3)$$

Equations 1 and 2 take the following forms:

$$\frac{1}{\tau^{M}}\frac{d}{dr}\left(\tau^{M}\frac{d\theta}{d\tau}\right)+\lambda(1+\varepsilon\theta)m_e{}^{\theta}/(1+\varepsilon\theta)-\delta\theta=0 \quad (4)$$

And boundary conditions are:

$$\frac{d\theta}{d\tau}(0)=0;\ \theta(1)=0 \quad (5)$$

Where:

θ = The dimensionless temperature
λ = The Frank-Kamenetskii parameter (reaction rate parameter)
ε = The activation energy parameter
τ = The dimensionless rectangular distance of the slab or radial distance of cylinder or sphere
δ = The dimensionless heat loss parameter

The dimensionless heat transfer rate at each medium's surface is expressed in terms of the Nusselt number as follows:

$$Nu=-\frac{d\theta}{d\tau}\ (\text{at } \tau=1) \quad (6)$$

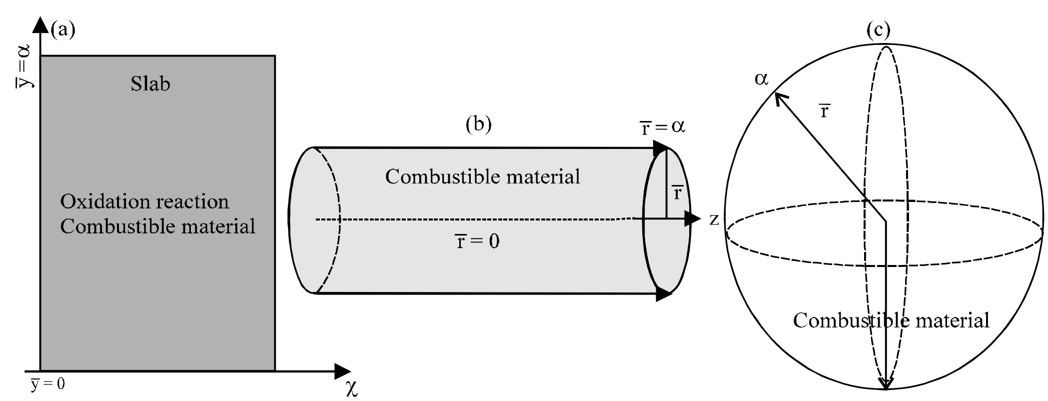

Fig. 1: The geometry of the problem for the: a) Slab; b) Cylinder and c) Sphere, respectively

Numerical algorithm: Equation 4 and 5 were solved using RKF45 method coupled with shooting technique. The algorithm gives results to expected accuracy. The following procedure is used where $0 = x_1$, $\theta' = x_2$. It becomes possible to transform Eq. 4 and 5 to first order differential equations as follows:

$$x_1' = x_2$$
$$x_2' = -\lambda(1+\varepsilon x_1)^m \exp\left(\frac{x_1}{1+\varepsilon x_1}\right)+\delta x_1 \quad (7)$$

The boundary conditions are expressed as:

$$x_1(0) = 0,\ x_2(0) = 1 \quad (8)$$

RESULTS AND DISCUSSION

In this study, we present computational results obtained for the model equations in the above section graphically and discuss the results quantitatively for various values of kinetic parameters embedded in the system.

Rate of reaction parameter (λ) on temperature profiles: We observe that an increase in λ results with a corresponding increase in temperature profiles (Fig. 2). In the slab, we experience the highest values of the temperature raise as λ is varied as compared to the cylinder and we see the lowest values of the temperature raise in the sphere. For example, at λ = 0.8, the temperature value in the slab is above 0.25 in the cylinder it is <0.25 but above 0.18 and in the sphere the temperature value is above 0.12 but <0.18. This shows that heat loss to the ambient is quicker in the sphere, followed by the cylinder and lastly, the slab. In other words, the sphere will take time to accumulate enough high temperatures that may lead to thermal runaway as compared to the cylinder and the slab.

Activation energy parameter (ε) on temperature profiles: We observe the same scenario that an increase in ε results with a corresponding increase in temperature profiles. We also observe that the temperature profiles for the slab are at highest values, with the highest value above 0.03 for the cylinder temperature profiles, the values are above 0.02 and below 0.03 and for the sphere the temperature profiles are just above 0.015 and below 0.02 (Fig. 3). The illustration confirms that the heat loss to the ambient on the sphere is the quickest compared to the cylinder and the slab.

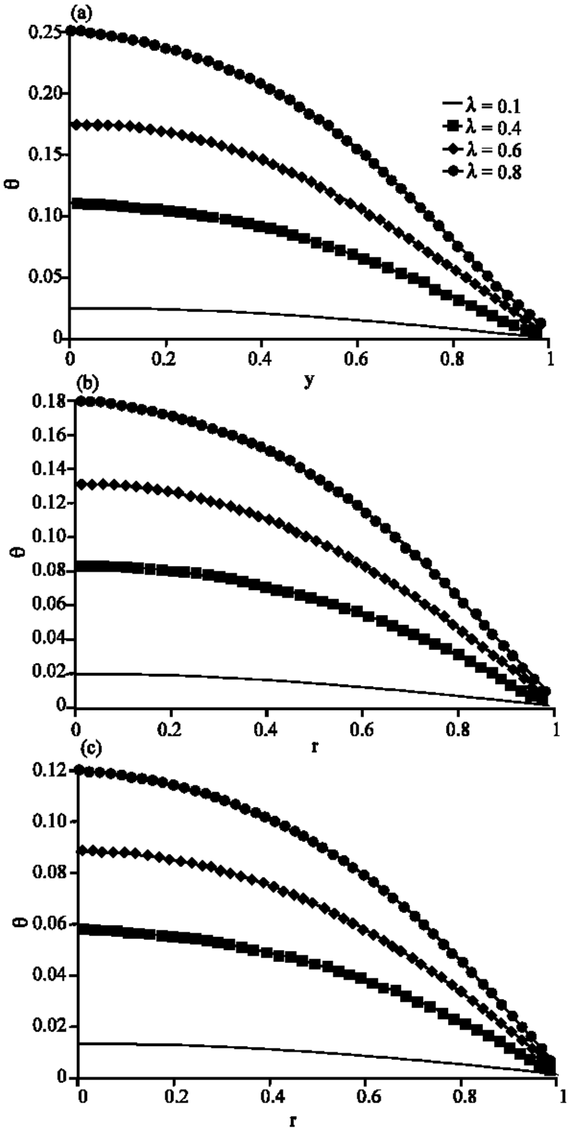

Fig. 2: Variation of λ with temperature in: a) Slab; b) Cylinder and c) Sphere respectively (m = 0.5, ε = 0.1, δ = 1)

Heat loss parameter (δ) on temperature profiles: In this case we observe effects of δ on the system's temperature behavior (Fig. 4). This is illustrated in temperature profiles. We also experience highest temperature profiles for the slab, the lowest for the sphere and the cylinder in the middle. The parameter δ facilitates loss of heat to the ambient especially at its highest values.

Numerical exponent (m) on temperature profiles: The numerical exponent takes the values -2, 0 and 0.5 as mentioned earlier. We see that an increase in m also corresponds to an increase in temperature profiles. It is worth noting that thermal ignition tends to occur in a

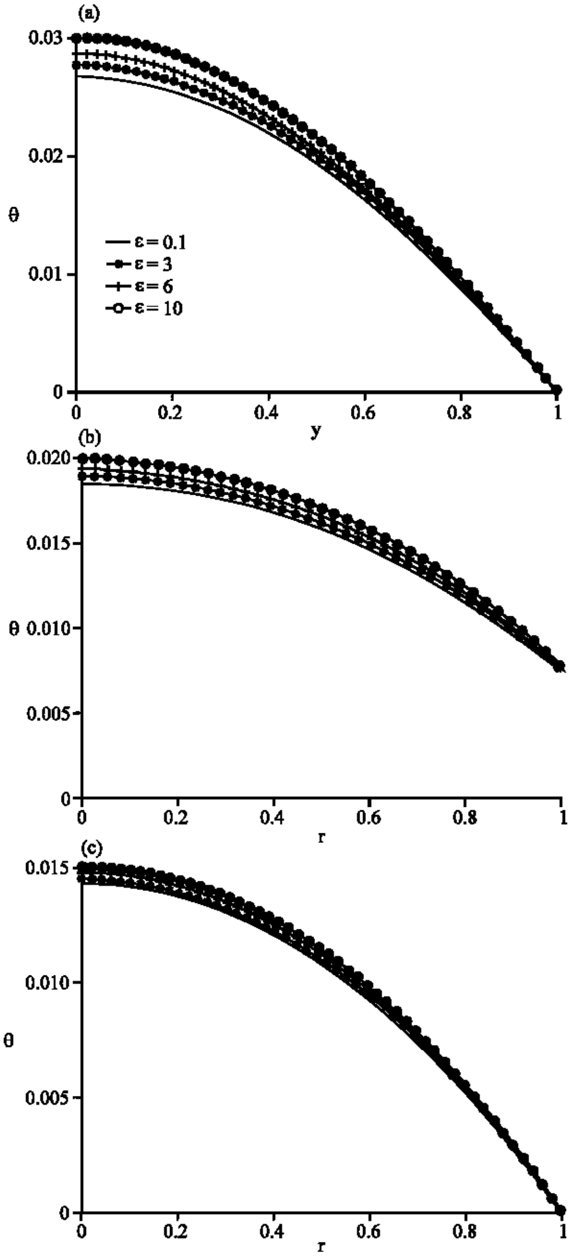

Fig. 3: a-c) Effects of variation on temperature (m = 0.5, ε = 0.1, δ = 1)

quicker way in biomolecular kinetics (m = 0.5) when compared to Arrhenius (m = 0) and sensitized (m = -2) kinetics. We observe the same trend that the temperature profiles are highest for the slab and lowest for the sphere (Fig. 5).

Thermal stability analysis: In this subsection, we investigate thermal stability in the slab, the cylinder and the sphere. This is done by plotting the Nusselt number

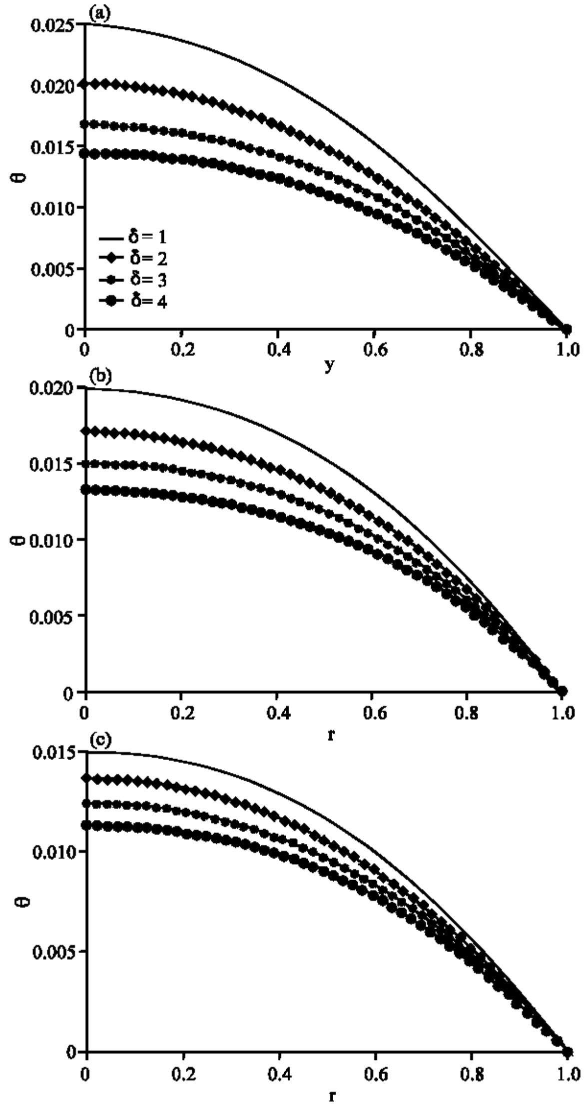

Fig. 4: a-c) An increase in results (m = 0.5, ε = 0.1, δ = 1)

(Nu) against the reaction rate parameter (λ). The results are presented graphically in Fig. 6-8 and are also expressed in Table 1.

Heat loss parameter (δ) variation: We see from Fig. 6a–c that an increase in δ gives a corresponding increase in Nu and λand. Thermal stability is indicated by larger values of λ or longest lines of the graph. We see for example, that the slab gives the lowest value of λ for which is 2.4676, the cylinder gives λ = 3.2428 and the sphere gives the highest value which is λ = 4.6458. This shows that the sphere has the most thermal stability and the cylinder has more thermal stability than the slab. Thermal stability is achieved at highest values of δ.

Table 1: Numerical values showing the effects δ, ε of and m on thermal criticality values

Parameters			Slab		Cylinder		Sphere	
δ	ε	m	Nu	λ	Nu	λ	Nu	λ
1	0.1	0.5	1.98338	1.7204	2.38761	2.5019	2.39524	3.9197
2	0.1	0.5	2.03732	2.0938	2.43287	2.8722	2.42995	4.2826
3	0.1	0.5	2.09084	2.4676	2.47558	3.2428	2.46169	4.6458
1	10	0.5	4.80782	3.0634	5.85083	4.4782	6.04731	7.1198
1	2.0	0.5	2.74296	2.2891	3.34845	3.3448	3.52342	5.3132
1	0.1	0.0	2.12650	1.8242	2.55856	2.6533	2.56740	4.1587
1	0.1	-2.0	3.06550	2.4297	3.70122	3.5387	3.70737	5.5635

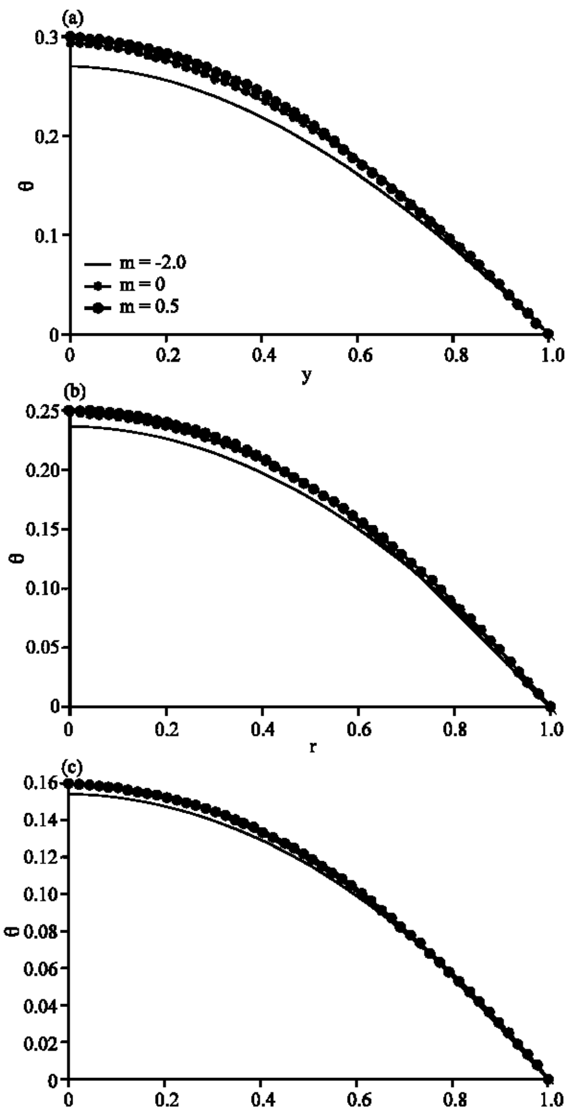

Fig. 5: a-c) The effects of different values of m on temperature profiles (λ = 0.5, ε = 0.1, δ = 1)

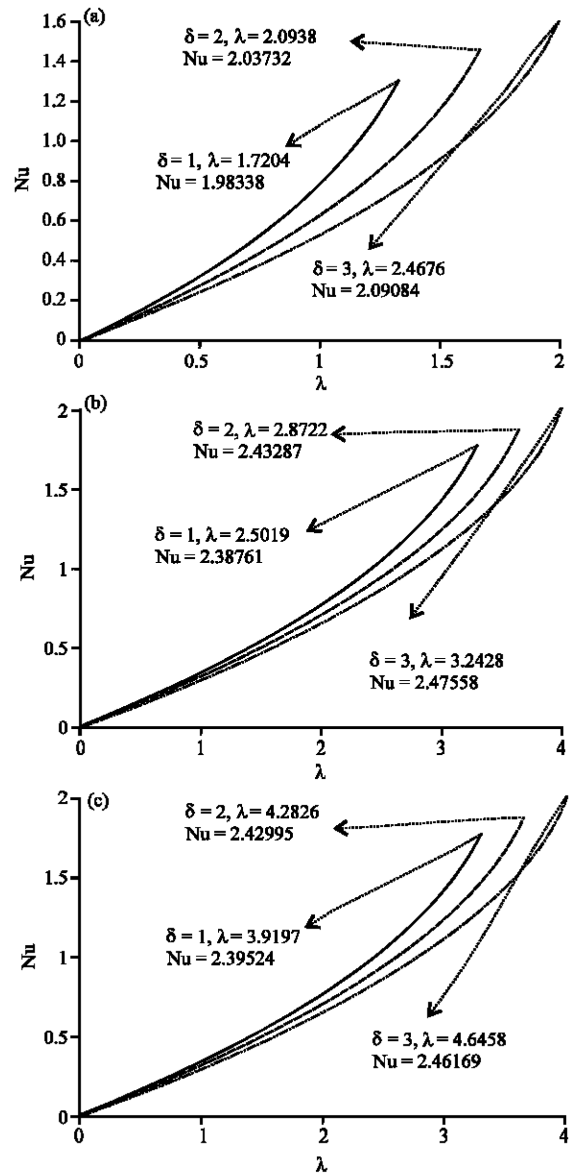

Fig. 6: a-c) Activation energy parameter (ε) variation

Numerical exponent (m) variation: In this case, we consider variation of m and its effect on thermal stability. An increase in m results with a decrease in Nu and λ values. Again, we see that thermal stability is highest in the sphere than in the cylinder and that the slab has the least thermal stability.

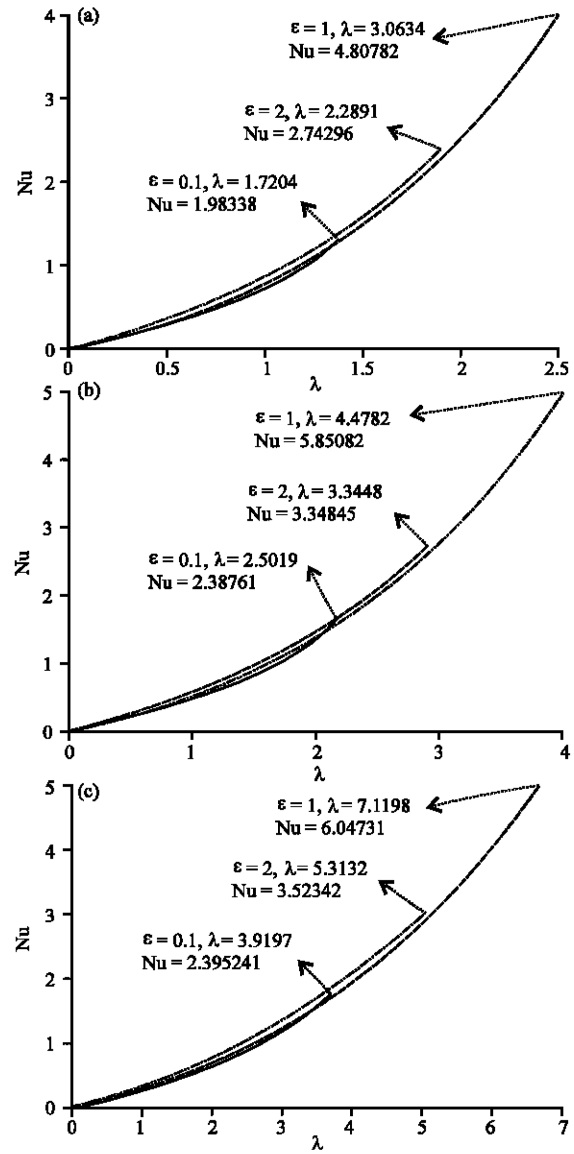

Fig. 7: a-c) Variation of and its effect on thermal stability of the system in each physical geometry

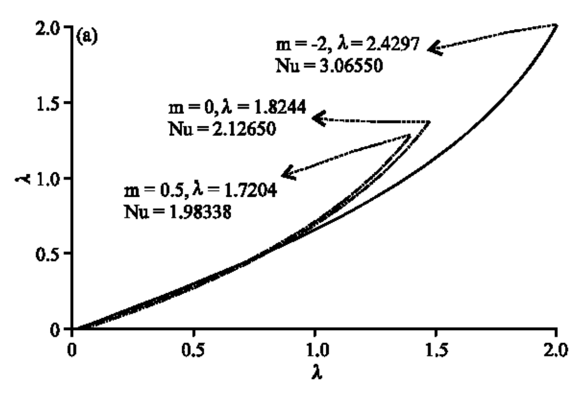

Fig. 8: Continue

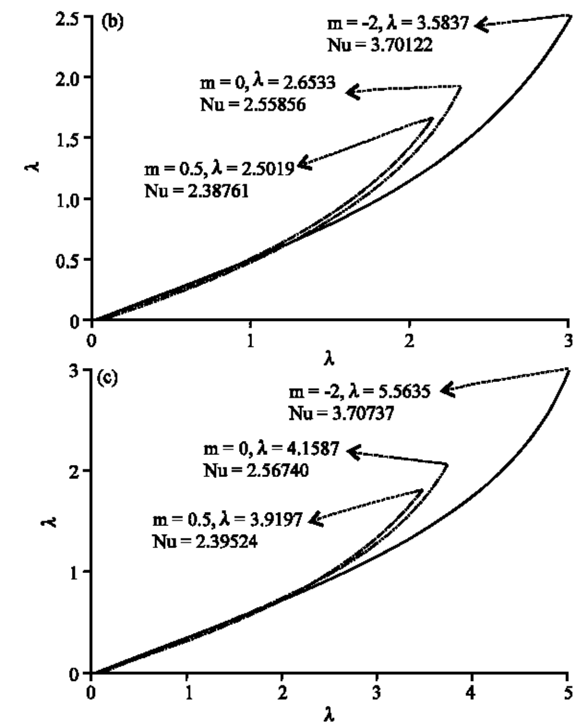

Fig. 8: a-c) Thermal stability is enhanced by keeping the lowest value of m

CONCLUSION

In this study, thermal stability was investigated simultaneously for media of different physical geometries. Kinetic parameters that enhance thermal stability are the ones which lower temperature profiles and in this case, we could identify δ as the parameter that enhances thermal stability. The main objective was to compare thermal stability in a slab, a cylinder and a sphere. The findings agree with the standard norm that the sphere has the most thermal stability and the cylinder has more thermal stability than the slab. It is a known phenomenon that heat transfer from a surrounding with highest temperature to a liquid inside a spherical container is lesser than that for a cylindrical vessel and least in a rectangular vessel. The main reason behind this is that a container in a spherical form has smaller surface area per unit volume than cylindrical and rectangular containers.

RECOMMENDATIONS

The significance of this study is to enhance packaging understanding of reactive material in appropriate physical geometry to allow safety and security. The investigation was done theoretically and the advantage is that the investigation without experimentation is quicker, safer and cheaper. This study can be extended to a situation where thermal conductivity varies with temperature of the system.

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