ON THE CRITICAL TEMPERATURE AND TRANSITIONAL VALUES OF A COMBUSTIBLE MIXTURE IN DIFFERENT MODES OF HEAT TRANSFER

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Abstract—In this study, the steady one-dimensional heat transfer process in a chemical substance, at rest in a vessel, involving branched-chain thermal reaction under generalized Arrhenius reaction-rate law is revisited. Two distinct boundary conditions are considered; constant surface temperature and Newton cooling on surface. The temperature equation and the specified boundary conditions are transformed into dimensionless forms for cartesian, cylindrical and spherical geometries. The developed non-linear equation is reduced to linear problem by assuming that the generalized heat generation term depends only on the maximum central dimensionless temperature. The resulting equations are then integrated analytically using standard techniques. The simplified yet accurate solutions obtained produces expressions for criticality condition and transition (disappearance of criticality). Comparison of present analytical expressions is in agreement with the limiting case of Arrhenius reaction-rate law. The analytical expressions obtained for criticality and transition conditions are shown graphically and discussed in detail for various parameters of interest.

Key Words and Phrases: Approximate analytical solutions, Branched-chain thermal reaction, criticality and transition conditions, Generalized Arrhenius reaction-rate law, Heat transfer process

1. Introduction

It is established in the literature (see [3], [12], [25]) that the dimensionless temperature formulation in combustion theory exists in two alternative dimensionless forms described as

$$\text{Case 1}: \ \phi = \frac{(T-T_a)E}{RT_a},$$
$$\text{Arrhenius term} = \exp\left(\frac{\phi}{1+\beta\phi}\right) \text{ and} \qquad (1)$$

$$\text{Case 2}: \ \theta = \frac{RT}{E}\left(\text{ or } = \frac{T}{T_a}\right),$$
$$\text{Arrhenius term} = \exp\left(-\frac{1}{\theta}\right) \cdot \left(\text{or} = \exp\left(-\frac{1}{\beta\theta}\right)\right). \qquad (2)$$

The two cases of nondimensionalization featured in mechanism of thermal theories of heat generation by chemical reaction, isothermal reacting flows or branched-chain theories as well as branched-chain thermal reaction. In these cicumstances the determination of critical and transitional values for thermal reaction problems is often of considerable interest. Accordingly, the emerging dimensionless measure here is the parameter $\beta = RT_a/E$. Furthermore, critical and transitional values for branched-chain thermal reactions in physical coordinates is quite common and may be obtained from results generated.

In this context, the dimensionless form

expressed in equation (1) has been extensively used to analysis combustible materials which takes account of thermal explosion and disapprarance of critical values for spatially distributed systems and unsteady scenarios. The earliest studies on the exact solution in the limit of $\beta = 0$ for spatially distributed models are the milestone papers by Frank-Kamenetskii [12] and Semenov [25]. Exact solutions were also obtained by Reddy [23] and Zeldovich et al. [30] under realistic assumptions while approximate solutions also exist (Boddington et al. [6], (Boddington et al. [7], (Boddington et al. [8] Makinde and Osalusi [14], Mustapha and Khaled [15], Okoya [16] and Okoya [20]). The problem of transient variation of temperature in reactor using equation (1) has been discussed under physically reasonable conditions by many researchers including Adegbie [1], Ayeni et al. [4], Luo et al. [13], Okoya [17], [18], [19]. It is note worthy that the dimensionless form of equation (2) has received little or no attention partly due to the advantage that the exponential heat source term allow for series approximation (see [27] for an example). However, considerable amount of qualitative information can be deduced when constant surface temperature are employed at the surface of the geometries. A steady state thermal explosion model was formulated under some realistic assumptions and solved employing the technique of upper and lower solutions by El-Sayed [9], [10], [11] and Shouman [26]. Shouman and Donaldson [27] as well as Adler [3] complemented the earlier researchers by obtaining series solutions and perturbation series expansion, respectively. In another important paper, Ponzio et al. [22] conducted experimental results, theoretical basis and generated a formular for prediction of ignition. Recently, Adebowale [2] studied an extended model using analytical technique with allowable dimensionless maximum temperature in the material. Although basic research on steady state thermal explosion using equation (2) have been conducted, however, the vast applicability of branched-chain thermal reactions in handling and storage of spontaneous exothermic reactions and materials suggests the need for further investigation. For practical purposes we investigate a particular problem arising from branched-chain thermal reaction using expression in equation (2) and subject to two different boundary conditions.

Therefore, this paper attempts to study approximate analytical solutions to the equations governing the heat transport process in a combustible mixture involving branched-chain thermal reaction at rest in a channel, cylinder and sphere geometries. The solutions for the dimensionless temperature distribution using the expression in (2) for each of the aforementioned geometries are presented and discussed. The effects of dimensionless ambient temperature, constant surface temperature and Newton cooling boundary conditions on the critical condition for explosion and extinction are analytically and numerically studied. Comparisons with known results in the literature is also carried out. The obtained results improve, complement and extend many results on branched-chain thermal explosion theory.

2. Mathematical problem formulation

Assuming that a combustible material at rest without reactant consumption is enclosed in a vessel. Such that an exothermic reaction based on the mixture of oxygen-acetylene and oxygen-hydrogen systems occur within the vessel under constant thermal initiation. No terms were added to describe the diffusion of the particles in line with the termination reaction adopted by [25]. By consideration of chemical kinetic and energy conservation equations, the generalized Arrhenius rate law for reaction branched-chain rate is assumed. It is also assumed that the temterature distribution is in a steady state. The equation of energy in the adiabatic isobaric system governing the heat flow for one-dimensional problem is given by (see [1], [17], [18], [19], [24], [28], [29], [30])

$$K\nabla^2 T + \alpha Q_0 \left(\frac{\kappa T}{\hbar \nu}\right)^m \left(\frac{T - T_a}{\alpha}\right)^n \exp\left(-\frac{E}{RT}\right) + \alpha A = 0. \quad (3)$$

Where the first term is diffusion of temperature, the second term indicates the chain branching heat production and the third term is the chain initiation.

Two relevant boundary conditions are considered below:

Model 1: Constant surface temperature at the wall

$$T(r = \pm b) = T_s, \quad \text{and} \quad (4)$$

Model 2: Newton cooling at the wall

$$K\frac{dT}{dr}(r = \pm b) = -H(T_s - T_a). \quad (5)$$

The boundary value problem formulations under these conditions is symmetric and this scenario was important for obtaining closed-form solution. Based on the scaling in the nomenclature, the dimensionless nonlinear equation and the associated boundary conditions are expressed in the form

$$\frac{d^2\theta}{dr^2} + \frac{j}{r}\frac{d\theta}{dr} + \delta\theta^m \left(\frac{\theta}{\beta} - 1\right)^n \exp\left(-\frac{1}{\theta}\right) + \epsilon = 0, \quad (6)$$

$$\theta(x = 1) = \theta_s, \quad \text{and} \quad \frac{d\theta}{dx}(x = 0);$$
$$\theta(0) = \theta_{max}, \text{ due to symmetry BC.} \quad (7)$$

and

$$\frac{d\theta}{dx}(x = 1) = -Bi(\theta_s - \theta_a), \quad and$$
$$\frac{d\theta}{dx}(x = 0);\ \theta(0) = \theta_{max},$$
$$\text{due to symmetry BC}. \quad (8)$$

Equations (6) - (8) cannot be solved analytically for θ due to the nonlinearity of the heat source term. However, simplifying assumption can be made on the source term to make the differential equation (6) trackable. In accordance with Shouman [26], it is assumed that the generalized heat generation source term is dependent only on the maximum central dimensionless temperature. In this wise, the differential equation (6) reduces to

$$\frac{d^2\theta}{dr^2} + \frac{j}{r}\frac{d\theta}{dr} + \delta\theta_{max}^m \left(\frac{\theta_{max}}{\beta} - 1\right)^n \cdot \exp\left(-\frac{1}{\theta_{max}}\right) + \epsilon = 0. \quad (9)$$

It is worth noting that θ_{max} is unknown at this stage but it can be assumed to be a constant.

2.1 Special models

For the purpose of comparison, the classical thermal equation of [27] is a special case of our model equation (6) if $\epsilon = m = n = 0$. Furthermore, the obtained classical thermal equation in [26] is a limiting scenario of the model equation (6) when $\epsilon = m = n = 0$ and simultaneously the problem reduces to that studied by [3] for $i = 0$. The corresponding classical thermal equation (3) for $A = n = 0$ was investigated by [8] and in [6] ($m = 0$ and $m = 1/2$), [11] ($m = -1$), [16] ($i = 0$ and $m = -2$). Equation (3) for branched-chain thermal reaction was originally formulated by [20] ($i = 0$) and [24] ($i = 1$).

2.2 Phenomenological models

We can directly integrate equation (9) twice, applying the boundary condition 7 (b) (or 8 (b)) and after some algebra the solution of the equation (9) becomes

$$\theta = \theta_{max} - \frac{x^2}{2(j+1)} \cdot \left[\delta\theta_{max}^m \left(\frac{\theta_{max}}{\beta} - 1\right)^n \exp\left(-\frac{1}{\theta_{max}}\right) - \epsilon\right]. \quad (10)$$

Next, we shall consider two sets of boundary conditions in order to investigate the criticality and transition of θ_s and θ_{max}. Firstly, we investigate the setup in case 1 where the surface temperature is set to a constant value and follow-up with the second case where a nonzero wall thermal flux condition is prescribed.

3. Case study 1: Constant surface temperature

Applying the boundary condition (7a) to the solution (10), we get

$$\theta_s = \theta(1) = \theta_{max} - \frac{1}{2(j+1)} \cdot \left[\delta\theta_{max}^m \left(\frac{\theta_{max}}{\beta} - 1\right)^n \exp\left(-\frac{1}{\theta_{max}}\right) - \epsilon\right]. \quad (11)$$

The nature of the temperature profile is obtained by studying equations (10) and (11) which can be combined to result in the form

$$\frac{\theta_{max}-\theta}{\theta_{max}-\theta_s} = x^2, \quad (12)$$

which produces parabolic distribution of temperature for all geometries, activation energy parameter and initiation rate constant.

Next we investigate the critical condition for equation (11). The mathematical expression for criticality is $d\delta/d\theta_{max} = 0$ and eliminating δ_{cr} from the result, we can find the final expression in the following form

$$\left(\frac{1-[m+n]}{\beta}\right)\theta_{max\ cr}^3 + \left[m - \frac{1}{\beta} - 1 + \frac{m+n}{\beta}\left(\theta_{s\ cr} - \frac{\epsilon}{2(j+1)}\right)\right] \cdot \theta_{max\ cr}^2 + \left[1 + \left(m - \frac{1}{\beta}\right)\left(\frac{\epsilon}{2(j+1)} - \theta_{s\ cr}\right)\right] \cdot \theta_{max\ cr} + \frac{\epsilon}{2(j+1)} - \theta_{s\ cr} = 0. \quad (13)$$

Two special cases can be deduced from model equation (13) which have closed-form solutions for criticality and transition while the third case is handled numerically.

3.1 Model 1

(a) $\boldsymbol{\beta \to \infty}$ and $\boldsymbol{\epsilon = 0}$

The simplest model available from equation (13) is when $\beta = 1/\epsilon \to \infty$ and this scenario was studied in [2]. Here, we give a short review of the results for comparison purposes. With this choice of $\beta \to \infty$ (i.e. very small activation energies) and $\epsilon = 0$ (absence of initiation rate constant) results in the process of purely thermal reaction and this leads to the problem of finding the two roots of

$$(m-1)\theta_{max\ cr}^2 + (1 - m\theta_{s\ cr})\theta_{max\ cr} - \theta_{s\ cr} = 0 \quad (14)$$

Using the above equation (14) one can easily calculate $\theta_{max\ cr}$, $\theta_{max\ tr}$, $\theta_{s\ cr}$ and $\theta_{s\ tr}$ as functions of m. Solving the resulting quadratic equation simplifies to the thermal explosion and extinction temperature,

$$\theta_{max\ cr} = \frac{(1-m\theta_{s\ cr}) \pm \sqrt{(1-m\theta_{s\ cr})^2 - 4(1-m)\theta_{s\ cr}}}{2(1-m)}, \quad m \neq 1, \quad (15)$$

where the solutions with the minus as well as plus signs before the square root correspond to the dimensionless thermal explosion and extinction, respectively. It is evident that the two curves merge into one transition point (i.e. the discriminant is zero), this point is often called the disappearance of criticality, when

$$(1 - m\theta_{s\ tr})^2 - 4(1-m)\theta_{s\ tr} = 0. \quad (16)$$

The above equation (16) yields

$$\theta_{s\ tr} = \begin{cases} 1/4 & m = 0, \\ \frac{2-m-2\sqrt{1-m}}{m^2} & m \neq 0. \end{cases} \quad (17)$$

and equation (15) reduces to

$$\theta_{max\ tr} = \frac{1-m\theta_{s\ tr}}{2(1-m)}, \quad m \neq 1. \quad (18)$$

Simplifying equation (18) using equation (17) result in

$$\theta_{max\ tr} = \begin{cases} \frac{1}{2} & m = 0, \\ \frac{m-1+\sqrt{1-m})}{m(1-m)} & m \neq 1. \end{cases} \quad (19)$$

It is easy to show from equation (19b) in the limit of $m \to 0$ that applying L'hospital rule corresponds to equation (19a). As $m = 0$ (Arrhenius case; $\theta_{s\ tr} = 1/4$ while $\theta_{max\ tr} =$

0.5) our results reduce to that given by [26] and for $\theta_{s\,tr} = 0$ the results reduces to [12] ($\theta_{max\,tr} = 0.5$).

(b) $m + n = 1$

We now consider the more interesting and general case in which the process is controlled by branched-chain thermal reaction. If $m + n = 1$ in equation (13) then the polynomial of degree three reduces to a quadratic equation that is amendable to closed-form solution. This leads to the problem of finding the two roots of:

$$\left[m - \frac{1}{\beta} - 1 + \frac{1}{\beta}\left(\theta_{s\,cr} - \frac{\epsilon}{2(j+1)}\right)\right]\theta_{max\,cr}^2 + \left[1 + \left(m - \frac{1}{\beta}\right)\left(\frac{\epsilon}{2(j+1)} - \theta_{s\,cr}\right)\right]\theta_{max\,cr} + \frac{\epsilon}{2(j+1)} - \theta_{s\,cr} = 0. \quad (20)$$

Clearly, the solution of equation (20) is

$$\theta_{max\,cr} = \frac{-[(m-1/\beta)P+1] \pm \sqrt{\{(m-1/\beta)P+1\}^2 - 4(m-1/\beta-1-P/\beta)P}}{2[m-1/\beta-1-P/\beta]}, \quad (21)$$

where $P(\epsilon, j, \theta_{s\,cr}) = \epsilon/2(j+1) - \theta_{s\,cr}$. For the prevalent case, $m + n = 1$, the negative sign in equation (21) corresponds to thermal explosion while the positive sign represents thermal extinction.

At transition point where the thermal explosion curve and thermal extinction curve coincides (i.e. disappearance of criticality) then satisfies

$$\theta_{max\,tr} = \frac{\left[\left(m-\frac{1}{\beta}\right)\left\{\frac{\epsilon}{2(j+1)} - \theta_{s\,tr}\right\} + 1\right]}{2\left[1 - m + \frac{1}{\beta} + \frac{1}{\beta}\left\{\frac{\epsilon}{2(j+1)} - \theta_{s\,tr}\right\}\right]}, \quad (22)$$

while

$$\theta_{s\,tr} = \frac{\epsilon}{2(j+1)} + \frac{2 - m + \frac{1}{\beta} - 2\sqrt{1-m}}{\left(m - \frac{1}{\beta}\right)^2 + \frac{4}{\beta}}. \quad (23)$$

Hence, $\theta_{max\,tr}$ in equation (22) is reduced to

$$\theta_{max\,tr} = \frac{\left(m-\frac{1}{\beta}\right)^2 + \frac{4}{\beta} - \left(m - \frac{1}{\beta}\right)\left(2 - m + \frac{1}{\beta} - 2\sqrt{1-m}\right)}{2\left[\left\{\left(m-\frac{1}{\beta}\right)^2 + \frac{4}{\beta}\right\}\left(1 - m + \frac{1}{\beta}\right) - \frac{1}{\beta}\left(2 - m + \frac{1}{\beta} - 2\sqrt{1-m}\right)\right]}. \quad (24)$$

It is note worthy that $\theta_{max\,tr}$ in equation (24) does not depend on initiation rate constant, ϵ and the geometric factor, j whereas the opposite is the case of $\theta_{s\,tr}$ in equation (23). Equation (24) or (23) for $\beta \to \infty$ and $\epsilon = 0$ reduces to the known results for the process of purely thermal explosion in equation (19) or (17). Therefore, equation (13) describes branched-chain thermal behaviour well over a fairly wide range of parameters.

(c) Numerical solution for $m, n \in \Re$

Unlike the previous problems, we cannot obtain exact solutions outside these ranges of parameters. The only feasible approach is to use computational analysis for the branched-chain thermal reaction problem defined in equation (13). In this study, the numerical techniques for finding roots of a polynomial of degree five developed by [21] was adopted for equation (13) on Maple 17 software system for various values of θ_s when other parameters are fixed. Since numerical methods are employed on equation (13) with three roots, one might expect errors in the choice of two relevant roots. For our investigation, we have employed the following parameter values except where stated as varying: $m = 0.3$, $n = 2$, $j = 1$, $Bi = \beta = 50$ and $\epsilon = 1$. In order to validate the results of the numerical computation, it is imperative to compare the numerical results with the exact solutions (23) and (24). For the established case of $m + n = 1$, the results of the present numerical calculations are tabulated against the exact solution in Table 1. Evidently, a very good agreement between the results was observed, which confirms the validity of the numerical approach.

TABLE 1

Comparison of exact solutions of $\theta_{max\ tr}$ and $\theta_{s\ tr}$ with numerics when $\epsilon = 10$, $\beta = 50$ and $j = 1$.

		$\theta_{max\ tr}$			$\theta_{s\ tr}$		
m	n	Exact	Present	Rel. Error	Exact	Present	Rel. Error
-2.0	3.0	0.21043546	0.21044525	$4.65X10^{-5}\%$	2.63361657	2.63361657	0 %
0.0	1.0	0.49504951	0.49507433	$5.01X10^{-5}\%$	2.74875622	2.74875622	0 %
0.25	0.75	0.61123745	0.61127375	$5.39X10^{-5}\%$	2.78554697	2.78554697	0 %
0.5	0.5	0.81492500	0.81494868	$2.91X10^{-5}\%$	2.84080682	2.84080682	0 %

Now, we turn our attention to the profile of $\theta_{max\ cr}$ versus $\theta_{s\ cr}$ as a function of n, m, β, ϵ and j so as to get physical insight. The results obtained by numerical computation are presented on variation of the dimensionless critical peak temperature, $\theta_{max\ cr}$ against the dimensionless critical surface temperature $\theta_{s\ cr}$ is displayed in Figures 1 - 5 for three values each of ϵ, β, j, m and n.

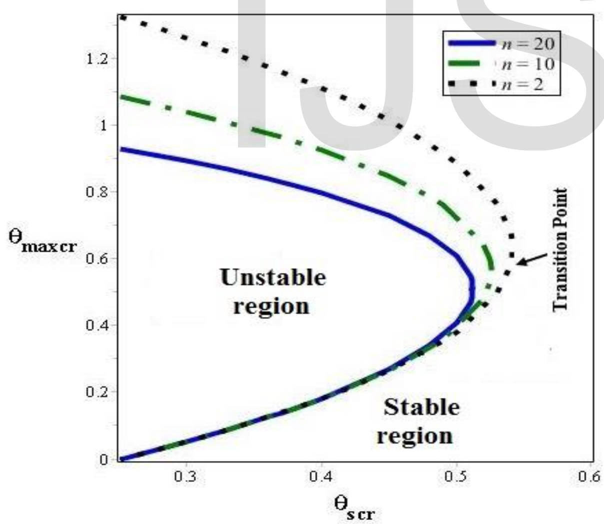

Figure 1: Solution curves of $\theta_{max\ cr}(\theta_{s\ cr})$ for various reaction order n as labelled.

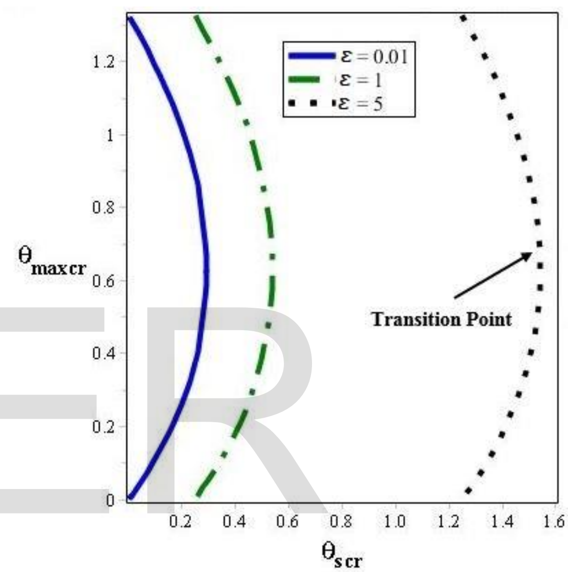

Figure 2: Solution plots of $\theta_{max\ cr}$ on $\theta_{s\ cr}$ for three values of initiation parameter, ϵ.

The results presented in Figures 1 - 5 show the influence of ϵ, β, j, m, n on $\theta_{max\ cr}$ against $\theta_{s\ cr}$. Four intructive properties are revealed for the process of branched-chain thermal reaction:

(i) It is evident that the dependence of $\theta_{max\ cr}$ on $\theta_{s\ cr}$ is continuous for various plots in Figures 1 - 5.

(ii) It can be seen that as ϵ, β and m increase the lower branch of the plots corresponding to thermal explosion increases while the higher branch of the plots decrease. The opposite behaviour is observed when j and n increase.

(iii) Also, it is shown that as n increase, the area under the curves corresponding to the critical region decrease while the increase in the parameters ϵ, β and m show the critical region increase. It is found that the area under the curves corresponding to the critical region for each geometry are in the order

$$\text{Area}_{cr}(\text{ sphere }) < \text{ Area}_{cr}(\text{ cylinder }) < \text{ Area}_{cr}(\text{ slab })$$

(iv) We noticed that in the graphical presentation of these results (Figures 1-5), discussion at transition is elusive. The result of the transitional values for the problem are appropriate in tabular form in order to capture the qualitative properties. With this in mind, Table 2 exhibit the dependence of emerging parameters at transition.

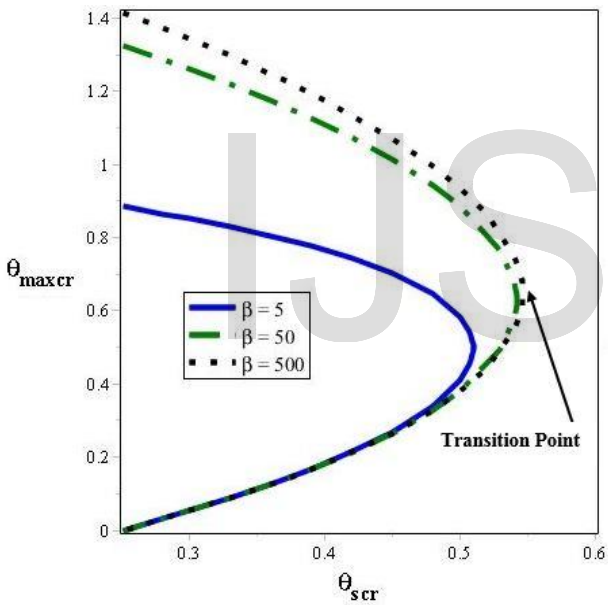

Figure 3: Plots of dependence of $\theta_{max\ cr}$ versus $\theta_{s\ cr}$ for values of activation energy parameter, β.

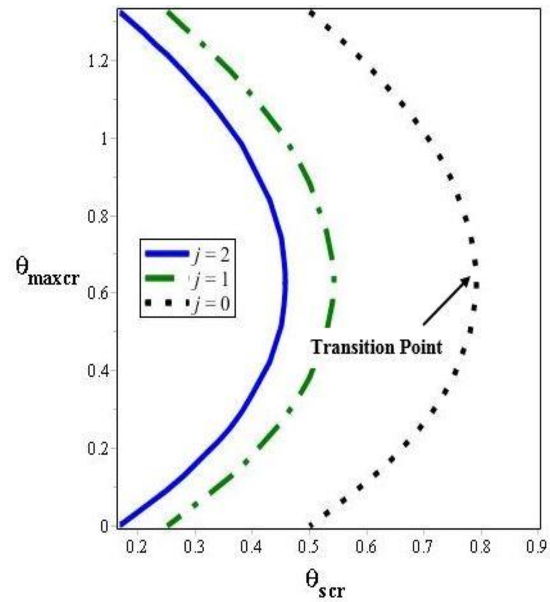

Figure 4: Graphical representation of $\theta_{max\ cr}$ against $\theta_{s\ cr}$ for systems of differing geometries, j.

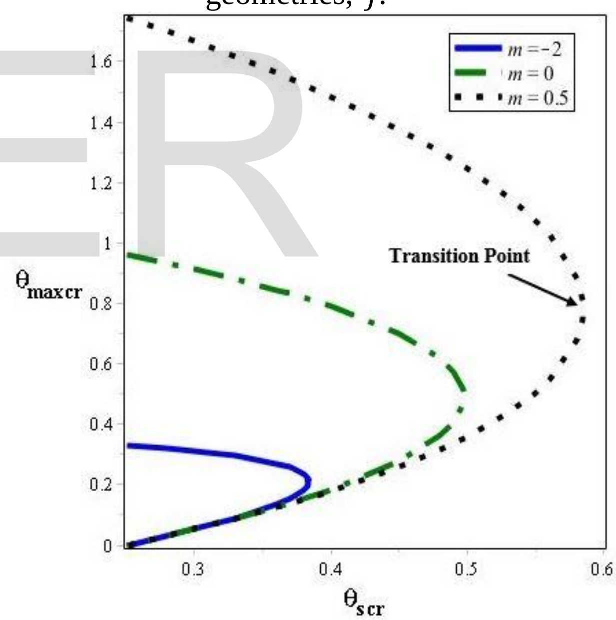

Figure 5: Behaviour of $\theta_{max\ cr}(\theta_{s\ cr})$ for different values of numerical exponent, m.

TABLE 2
The transitional values of branched-chain thermal mechanisms deduced from the above figures.

ϵ	β	j	m	n	$\theta_{max\,tr}$	$\theta_{s\,tr}$
0.001					0.6281129	0.2941166
1	50	1	0.3	2	0.6281129	0.5416165
5					0.6281524	0.5416165
	5				0.4993742	0.5093589
1	50	1	0.3	2	0.6281129	0.5416166
	500				0.6483661	0.5459437
		0			0.6281129	0.7916166
1	50	1	0.3	2	0.6281129	0.5416166
		2			0.6281058	0.4582832
			-2		0.2107605	0.3837354
1	50	1	0	2	0.4903297	0.4975485
			05		0.7798154	0.5843766
				2	0.6281129	0.5416165
1	50	1	0.3	10	0.5625877	0.5260944
				20	0.5098191	0.5117865

The first block of rows of the table indicates that as ϵ increases the $\theta_{max\,tr}$ remains almost constant in the range of values whereas there is small increase in$\theta_{s\,tr}$ but it is asymptotic. This is to be expected since in practice, the parameter ϵ is small and an increase in ϵ indicates the effect of initiation of radicals becoming less significant. The next block of rows of the table shows the influence of β at transition. We observe that when β increased, both $\theta_{max\,tr}$ and $\theta_{s\,tr}$ increase. It is observed from the third block of rows that as j increases the $\theta_{max\,tr}$ remains almost constant while the $\theta_{s\,tr}$ decreases. The fourth (or last) block of rows reveals that as m (or n) increases, there is a tremendous increase (or decrease) in both $\theta_{max\,tr}$ and $\theta_{s\,tr}$.

Similarly, the second boundary condition can be discussed in an equally simple manner.

4. Case study 2: Convective cooling

Using the convectionally cooled boundary condition (8) to the solution (10), we obtain

$$\theta_a = \theta_s - \frac{1}{(j+1)Bi} \cdot\left[\delta\theta_{max}^m\left(\frac{\theta_{max}}{\beta}-1\right)^n \exp\left(-\frac{1}{\theta_{max}}\right)-\epsilon\right]. \quad (25)$$

Eliminating θ_s by substituting equation (11) into equation (25) gives

$$\theta_a = \theta_{max} - \frac{(2+Bi)}{2(j+1)Bi} \left[\delta\theta_{max}^m\left(\frac{\theta_{max}}{\beta}-1\right)^n \exp\left(-\frac{1}{\theta_{max}}\right)-\epsilon\right]. \quad (26)$$

The critical condition for thermal explosion (maximum)and extinction (minimum) can be obtained from equation (26) by setting $d\delta/d\theta_{max}=0$, which gives

$$\frac{2(j+1)Bi}{(2+Bi)} = \delta_{cr}\theta_{max\,cr}^{m-2} \cdot\left(\frac{\theta_{max\,cr}}{\beta}-1\right)^n \exp\left(-\frac{1}{\theta_{max\,cr}}\right) \cdot\left(m\theta_{maxcr}+\frac{n\theta_{max\,cr}^2}{\beta(\theta_{max\,cr}/\beta-1)}+1\right) \quad (27)$$

Utilizing equations (26) in equation (27), the critical dimensionless temperature can be expressed in terms of θ_a as

$$1 = \frac{\left(\theta_{max\,cr}-\theta_a+\frac{\epsilon(2+Bi)}{2(j+1)Bi}\right)\left(m\theta_{max\,cr}+n\frac{\theta_{max\,cr}^2}{\beta(\theta_{max\,cr}/\beta-1)}+1\right)}{\theta_{max\,cr}^2}. \quad (28)$$

Expanding equation (28) and collecting coefficients of powers of $\theta_{max\,cr}$ gives

$$\left(\frac{1-[m+n]}{\beta}\right)\theta_{max\,cr}^3 + \left[m-\frac{1}{\beta}-1+\frac{m+n}{\beta}\left(\theta_a-\frac{\epsilon(2+Bi)}{2(j+1)Bi}\right)\right] \cdot\theta_{max\,cr}^2 + \left[1+\left(m-\frac{1}{\beta}\right)\left(\frac{\epsilon(2+Bi)}{2(j+1)Bi}-\theta_a\right)\right]$$

$$\cdot\, \theta_{max\ cr} + \frac{\epsilon(2+Bi)}{2(j+1)Bi} - \theta_a = 0. \qquad (29)$$

The equivalent of equation (29) in terms of θ_s can be obtained as follows: substituting equation (25) into equation (27) and carrying out the elementary simplification, we have

$$\frac{2}{Bi+2} = \frac{\left(\theta_{s\ cr} - \theta_a + \frac{\epsilon}{(j+1)Bi}\right)\left(m\theta_{max\ cr} + n\frac{\theta_{max\ cr}^2}{\beta(\theta_{max\ cr}/\beta - 1)} + 1\right)}{\theta_{max\ cr}^2}. \qquad (30)$$

Eliminate θ_a by subtracting equation (30) from equation (28), we readily obtain

$$\frac{Bi}{2+Bi} = \frac{\left(\theta_{max\ cr} - \theta_{s\ cr} + \frac{\epsilon}{2(j+1)}\right)\left(m\theta_{max\ cr} + n\frac{\theta_{max\ cr}^2}{\beta(\theta_{max\ cr}/\beta - 1)} + 1\right)}{\theta_{max\ cr}^2}, \qquad (31)$$

which after rearranging corresponds to

$$\left(\frac{\frac{Bi}{2+Bi} - [m+n]}{\beta}\right)\theta_{max\ cr}^3 + \left[m - \frac{1}{\beta} - \frac{Bi}{2+Bi} + \frac{m+n}{\beta} \cdot \left(\frac{\epsilon}{2(j+1)} - \theta_{s\ cr}\right)\right]\theta_{max\ cr}^2 + \left[1 + \left(m - \frac{1}{\beta}\right)\left(\frac{\epsilon}{2(j+1)} - \theta_{s\ cr}\right)\right]\theta_{max\ cr} + \frac{\epsilon}{2(j+1)} - \theta_{s\ cr} = 0. \qquad (32)$$

The setup described in the model equations (29) and (32) can be solved analytically for some special cases otherwise numerically. We shall start with analytical solution for two special cases.

4.1 Model 2

(a) $\beta = \infty$ and $\epsilon = 0$

This special model was investigated in [2]. Here, we give a short review of the results for completeness. Equations (29) and (32) as well as the assumption that $\beta = 1/\epsilon \to \infty$, reduce to

$$(m-1)\theta_{max\ cr}^2 + (1 - m\theta_a)\theta_{max\ cr} - \theta_a = 0, \qquad (33)$$

and

$$\left(m - \frac{Bi}{2+Bi}\right)\theta_{max\ cr}^2 + (1 - m\theta_{s\ cr})\theta_{max\ cr} - \theta_{s\ cr} = 0. \qquad (34)$$

The dimensionless temperature values at criticality (negative sign for thermal explosion and positive sign for extinction) can be expressed as function of ambient and constant surface temperature by solving equations (33) and (34), respectively reduce to

$$\theta_{max\ cr} = \frac{(1 - m\theta_a) \pm \sqrt{(1 - m\theta_a)^2 - 4(1-m)\theta_a}}{2(1-m)}, \quad m \neq 1, \qquad (35)$$

and

$$\theta_{max\ cr} = \frac{(1 - m\theta_{s\ cr}) \pm \sqrt{(1 - m\theta_{s\ cr})^2 - 4\left(\frac{Bi}{2+Bi} - m\right)\theta_{s\ cr}}}{2\left(\frac{Bi}{2+Bi} - m\right)}, \quad m \neq \frac{Bi}{2+Bi}. \qquad (36)$$

Substitution of equation (35) with the minus sign (explosion) into equation (34) obviously produces the surface temperature at explosion as a function of the ambient temperature i.e.

$$\theta_{s\ cr} = \frac{4 + 2[2m(m-3) + Bi(m^2 - 3m + 2)]\theta_a + 2m^2 D_1\theta_a^2 + D_2(\theta_a; m, D_1)}{4(1-m)^2(2+Bi)\left(1 + \frac{m}{2(1-m)}\left\{1 - m\theta_a - \sqrt{(1-m\theta_a)^2 - 4(m-1)\theta_a}\right\}\right)}, \qquad (37)$$

where $D_1 = 2m + (m-1)Bi$ and $D_2 = (-4 + 2mD_1\theta_a)\sqrt{(1 - m\theta_a)^2 - 4(m-1)\theta_a}$.

It can be seen from equation (35) that at transition the discriminant is zero i.e.

$$\theta_a = \begin{cases} 1/4 & m = 0, \\ \frac{2 - m - 2\sqrt{1-m}}{m^2} & m \neq 0. \end{cases} \qquad (38)$$

It is interesting to note that at transition, θ_a in equation (17) and θ_a in equation (38) are identical in the limit of $Bi \to \infty$. On appealing to equation (38), it is evident that equation (37) after some algebra reduces to the transitional dimensionless surface temperature for the branched-chain thermal reaction i.e.

$$\theta_{s\,tr} = \begin{cases} \dfrac{4+Bi}{4(2+Bi)} & m = 0, \\[2ex] \dfrac{8m-8Bi(1-m)-4\{2m+Bi(m-2)\}\sqrt{1-m}}{4(2+Bi)m^2\sqrt{1-m}} & m \neq 0, 1. \end{cases} \quad (39)$$

It is worth noting that the results for $m = 0$ in equation (38) and (39) are obtained by applying L'Hospital rule twice and they correspond to the result in [26]. Evidently, the constant surface temperature scenario is equal to the convective scenario in the limit of $Bi \to \infty$ for which θ_a and θ_s are identical. A similar argument supports this well-known fact in [26]. It is also important to note that in the event with $Bi \to \infty$ in equation (39) and $\theta_{s\,tr}$ in equation (17) are identical establishing that in this special case the constant surface temperature and Newtonian convecting cooling at the walls are equivalent. Moreover, when $m + n = 1$ and $m + n = Bi/(2 + Bi)$ in equations (29) and (32), respectively, scenarios which clearly reduces to special cases with analytical solutions, will be tackled in the next subsection.

(b) $m + n = 1$ and $m + n = Bi/(2 + Bi)$

Firstly, as $m + n = 1$, it is apparent that equation (29) for convective cooling is similar to equation (20) for constant surface temperature, if we replace P with $H(Bi, \epsilon, j, \theta_{s\,cr}) = \epsilon(2 + Bi)/[2Bi(j + 1)] - \theta_a$. Hence, the results for criticality and transition for convective cooling case can be adapted in order to save space.

Secondly, for m and n satisfying $m + n = Bi/(2 + Bi)$, equation (32) permits the solution

$$\theta_{max\,cr} = \frac{-[(m-1/\beta)P+1] \pm \sqrt{\{1-(m-1/\beta)P\}^2+4Bi(1+P/\beta)/(2+Bi)]P}}{2[m-1/\beta-Bi(1+P/\beta)/(2+Bi)]}. \quad (40)$$

Proceeding in the usual manner, the transitional values for θ_{max} and θ_s for the convective cooling readily results in

$$\theta_{max\,tr} = \frac{\left[\left(m-\frac{1}{\beta}\right)\left\{\frac{\epsilon}{2(j+1)}-\theta_{s\,tr}\right\}+1\right]}{2\left[\frac{Bi}{2+Bi}-m+\frac{1}{\beta}+\frac{Bi}{(2+Bi)\beta}\left\{\frac{\epsilon}{2(j+1)}-\theta_{s\,tr}\right\}\right]}, \quad (41)$$

and

$$\theta_{s\,tr} = \frac{\epsilon}{2(j+1)} + \frac{\frac{2Bi}{2+Bi}-m+\frac{1}{\beta}-2\sqrt{\frac{Bi}{2+Bi}\left(\frac{Bi}{2+Bi}-m\right)}}{\left(m-\frac{1}{\beta}\right)^2+\frac{4Bi}{\beta(2+Bi)}}. \quad (42)$$

If we substitute equation (42) into equation (41) and simplifying, then $\theta_{max\,tr}$ is given by

$$\theta_{max\,tr} = \frac{\left(m-\frac{1}{\beta}\right)^2+\frac{4}{\beta}-\left(m-\frac{1}{\beta}\right)\left(2-m+\frac{1}{\beta}-2\sqrt{1-m}\right)}{2\left[\left\{\left(m-\frac{1}{\beta}\right)^2+\frac{4}{\beta}\right\}\left(\frac{Bi}{2+Bi}-m+\frac{1}{\beta}\right)-\frac{Bi}{\beta(2+Bi)}\left(2-m+\frac{1}{\beta}-2\sqrt{1-m}\right)\right]}. \quad (43)$$

Evidently, taking $Bi \to \infty$, it follows that $\theta_{max\,tr}$ and $\theta_{s\,tr}$ from equations (41) - (43) thereby reduce to equations (22) - (24), respectively.

Having now found $\theta_{max\,cr}$ and $\theta_{s\,cr}$ in subsections (a) and (b) for the parameter regions, the two special cases studied for the convective cooling are slightly restrictive. The focus of the next subsection is on parameter sensitivity using numerical computation in view of the fact that equation (32) cannot be further tackled analytically.

(c) Numerical solution for $m, n \in \mathfrak{R}$

Here we discuss the numerical solutions of equations (29) and (32). Firstly, we consider equation (32) and study the nature of the solution. It is worth noting that equation (32) is different from that given in equation (13) due to the term associated with the Biot number Bi. In fact, in the limit of $Bi \to \infty$ in equation (32), we would recover equation (13). The result for the convective boundary condition is different from that of the constant surface temperature in scale but not in the purpose it serves. Since the effects of m , n , β , ϵ and j on the distributions of the criticality and transition of dimensionless temperature were reported early, we will look only at the effect of parameter Bi. The variation of $\theta_{max\ cr}$ with the $\theta_{s\ cr}$ for the branched-chain thermal explosion regime is displayed in Figure 6. It is evident that the dependence of $\theta_{max\ cr}$ on $\theta_{s\ cr}$ is continuous as portrayed in Figures 6. Also, The lower branch of the plot in Figure 6 represents thermal explosion and the higher branch of the graph represents extinction. The two branches coincides at one point (transition point) after which critical value disappears. In adition, the unstable plane decreases with increasing Biot number.

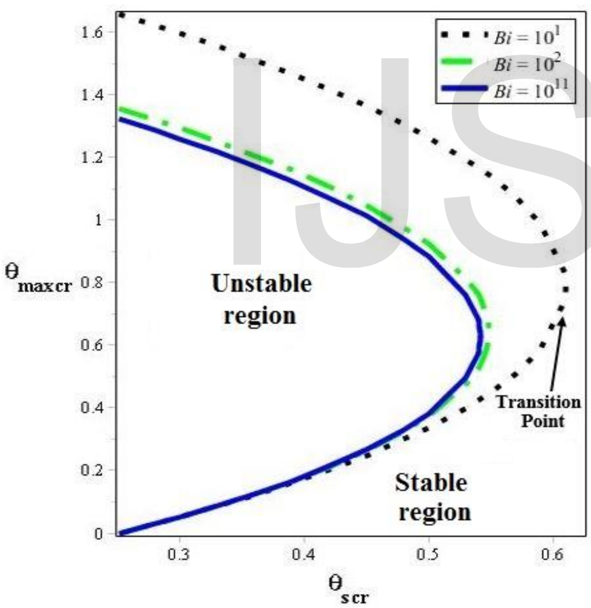

Figure 6: Shape of $\theta_{max\ cr}$ against $\theta_{s\ tr}$ for three values of Biot number, Bi.

To show the effects of transitional values, the numerical study that follows focus on transition values for the convective case using equation (32). It covers the complete range of values for Bi which can vary from 0 to ∞ as contained in Table 3. The table provides an independent check on the convergence of the solutions to eight decimal places.

TABLE 3

The transitional values of branched-chain thermal mechanisms partly deduced from the Figure 6.

Bi	$\theta_{max\ tr}$	$\theta_{s\ tr}$
0	8.61141234	8.86142000
10^0	2.39844456	1.35093291
10^1	0.78660349	0.61076463
10^2	0.64343981	0.54836438
10^5	0.62807920	0.54162330
10^7	0.62806414	0.54161664
10^9	0.62804586	0.54161657
10^{10}	0.62803641	0.54161657
10^{11}	0.62803778	0.54161657
10^{12}	0.62803778	0.54161657

It is revealed in Table 3 that as Bi increases, $\theta_{max\ tr}$ and $\theta_{s\ tr}$ decrease. It is worth noting that the solutions for both $\theta_{max\ tr}$ and $\theta_{s\ tr}$ in the limit of $Bi \rightarrow \infty$ for Table 3 agree with the corresponding solutions in the second block of rows in Table 2.

Secondly, we turn our attention on equation (29) for which $\theta_{max\ cr}$ is a function of θ_a. The general model given by equation (29) will be studied for regime of emerging parameters. In this case, we further present computational analysis of the branched-chain thermal reaction as portrayed in the Figures 7 - 11.

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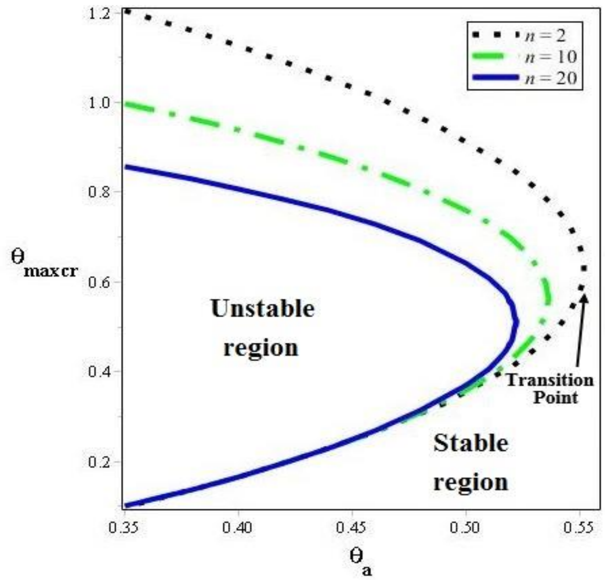

Figure 7: Solution curves of $\theta_{max\ cr}$ (θ_a) for various reaction order n as labelled.

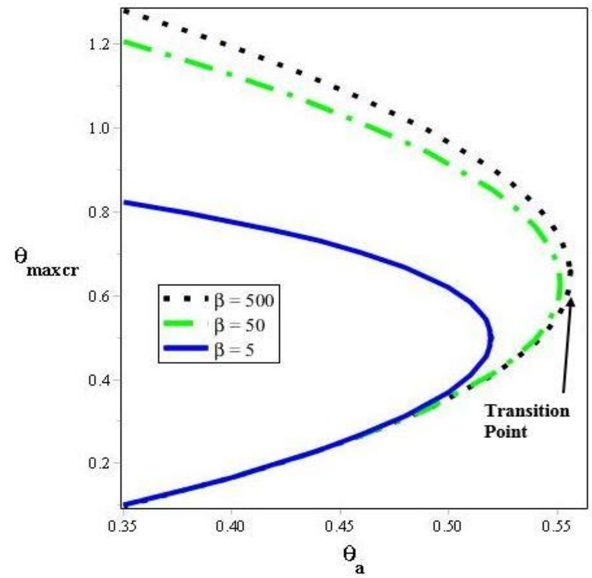

Figure 9: Plot of $\theta_{max\ cr}$ versus θ_a for various systems with values of activation energy parameter, β.

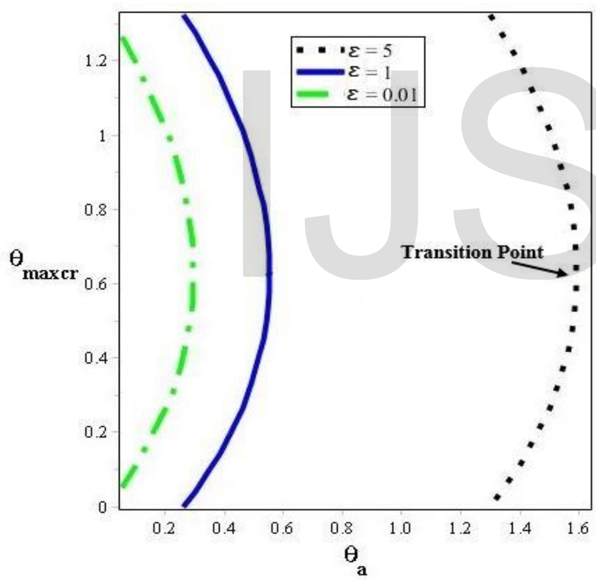

Figure 8: Graphs of $\theta_{max\ cr}$ as a function θ_a for three values of initiation parameter, ϵ.

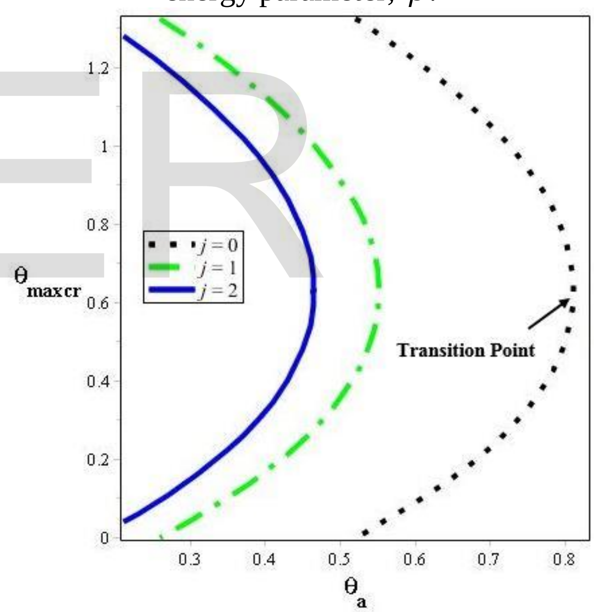

Figure 10: Effect of $\theta_{max\ cr}$ against θ_a for systems of differing geometries, j.

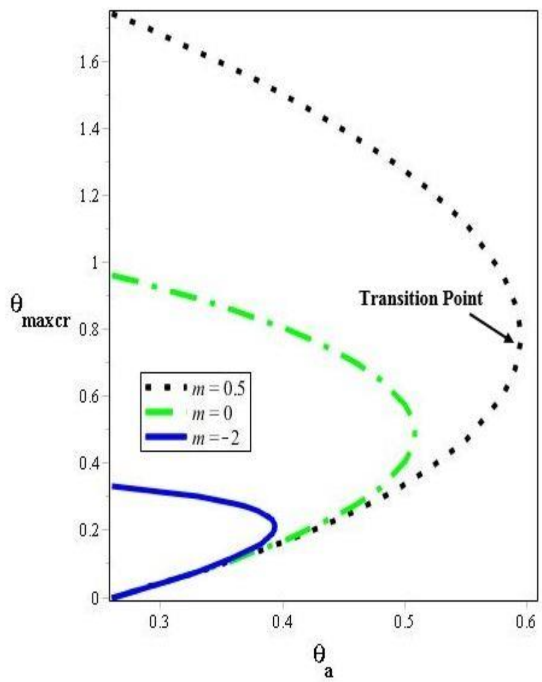

Figure 11: Variation of $\theta_{max\ cr}$ with θ_a for different values of numerical exponent, m

The results displayed in Figures 7 - 11 show the predicted variation of dimensionless critical peak temperature $,\theta_{max\ cr}$ with respect to dimensionless ambient temperature, θ_a for various values of ϵ, β, j, m and n. The following properties can be deducted from Figures 6 - 11:

(i) It is clearly seen from Figures 6 - 11 that the dependence of $\theta_{max\ cr}$ on θ_a is a continuous function.

(ii) The important features of the control parameters (lower branch of the plots corresponding to thermal explosion) in the present section is similar in result to that of the previous section.

(iii) Also, the parameter variation (area under the curves corresponding to the critical region) in the present section markedly reflect the same result as in the previous section. (iv) In order to better understand the transitional values for the problem a tabular presentation of the results in Figures 6 - 11 was generated using additional computations.

Table 4 shows the results of the root finding of equation (29) in the form of $\theta_{max\ tr}$ as a functions of θ_a for various values of ϵ, β, Bi, j, m and n.

TABLE 4

The transitional values of branched-chain thermal mechanisms deduced from Figures 7-11

.

ϵ	β	Bi	j	m	n	$\theta_{max\ tr}$	θ_a
0.01						0.62803777	0.29421657
1	50	50	1	0.3	2	0.62803777	0.55161657
5						0.62803777	1.59161657
	5					0.49928814	0.51935889
1	50	50	1	0.3	2	0.62803777	0.55161657
	500					0.64832006	0.55594374
		5				0.62803777	0.64161657
1	50	50	1	0.3	2	0.62803777	0.55161657
		500				0.62803777	0.54262657
			0			0.62803777	0.81161657
1	50	50	1	0.3	2	0.62803777	0.55161657
			2			0.62805750	0.46494991
				-2		0.21071772	0.39373536
1	50	50	1	0	2	0.49030736	0.50754855
				05		0.77963159	0.59437663
					2	0.62803777	0.55161657
1	50	50	1	0.3	10	0.56253901	0.53609438
					20	0.50979347	0.52178646

Table 4 illustrates the effect of different physical parameter of interest on the transitional values of the dimensionless central temperature, $\theta_{max\ tr}$ and ambient temperature, θ_a . The numerical exponent of the pre-exponential factor (m), dimensionless measure of the activation energy (β) increase the value of $\theta_{max\ tr}$ and θ_a whereas the value of branched-chain thermal reaction order (n) decreases the value of $\theta_{max\ tr}$ and θ_a . Furthermore, the initiation rate constant (ϵ) and Biot number (Bi) did not have any effect on the $\theta_{max\ tr}$ while geometric factor marginally increase $\theta_{max\ tr}$. θ_a increases when the initiation rate constant (ϵ) increases but θ_a decreases as Biot number (Bi) and geometric factor (j) increase.

the following:

1. The behaviour of solutions for $\theta_{max\ cr}(\theta_{s\ cr})$ for the dimensionless constant surface temperature and Newton cooling on the surface as well as $\theta_{max\ cr}(\theta_a)$ for the Newton Cooling on the surface is similar but differ in

5. Conclusion

In the present article, we have studied the steady state reaction involving branched-chain thermal systems and generalized Arrhenius kinetics using analytical and numerical methods with allowable dimensionless maximum temperature for the material source term. New exact analytical solutions for the two problems of constant surface temperature and convective cooling were studied for the infinite slab, infinite cylinder and sphere. Where there is common ground, agreement is excellent. We further implemented numerical investigation of the branched-chain thermal reaction. Hence, based on this analysis and the values of the dimensionless parameters investigated, we state

magnitude.

2. The results were validated for the dimensionless constant surface temperature and Newton cooling on the surface by comparing the classical analytical solutions with our solution when $n \to 0$, $Bi \to \infty$ and $\theta_{s\ tr} \to 0$.

3. The value of both $\theta_{max\,tr}$ and $\theta_{s\,tr}$ depend strongly on the activation energy parameter β, the numerical exponent of the pre-exponential factor m and branched-chain thermal reaction order n.

4. The profile for the variation of $\theta_{max\,cr}$ against the emerging parameters for the constant surface temperature and convectionally cooled boundary condition is similar in form but they are very dissimilar in scale.

5. The numerical treatment is valid for arbitrary Biot number.

6. The results obtained in [26] for the classical case (thermal reaction) under constat surface temperature and convectionally cooled boundary condition can be recovered easily when $m, n, \epsilon \to 0$.

NOMENCLATURE

Alphabets

A	initiation rate which is assumed constant during an explosion
b	half -width of the channel or radius
BC	boundary condition
Bi	$= bH/K$, Biot number
C_p	heat capacity at constant pressure
j	= geometric factor equal to 0, 1 and 2 for channel, cylinder and sphere, respectively
K	diffusion coefficient
m	numerical exponent of the pre-exponential factor
n	branched-chain thermal reaction order
Q_0	mth order rate constant for branched-chain
Q_f	energy released in the process per mole of fuel consumed by the mixture
r	radial distance
R	Universal gas constant
T	temperature of the vessel
T_a	constant ambient temperature
T_s	constant surface temperature
x	dimensionless radial distance

Greek Symbols

α	$= Q_f/(\rho C_p)$,
β	$= RT_a/E$, dimensionless measure of the activation energy
ϵ	$= b^2 A\alpha\beta/(DT_a)$, initiation rate constant
δ	$= \beta B_0 b^2 \alpha(\kappa T_a/(\beta\nu\hbar))^m (T_a/\alpha)^n/(DT_a)$, Frank Kamenetskii parameter
θ	$= RT/E$, dimensionless temperature of the model vessel
θ_a	$= RT_a/E$, constant dimensionless ambient temperature
θ_s	$= R_s T/E$, constant dimensionless surface temperature
$\hbar$	Planck's number
ν	vibration frequency
κ	Boltzmann constant
ρ	density of the mixture

Subscripts and superscripts

a	pertaining to ambient temperature
cr	critical value
max	maximum
s	surface
tr	transitional

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