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Criticality and Thermal Distribution of Combustion-Reaction in a Concentric Cylinder with Heat Loss and Bimolecular Kinetics

T. O. Sarumo[1*]; R. A. Oderinu[2]; S. O. Salawu[3]

[1]Department of Mathematics, Federal College of Education (Special), Oyo, Nigeria
[2]Department of Pure and Applied Mathematics, Ladoke Akintola University of Technology, Ogbomoso, Nigeria
[3]Department of Mathematics, Bowen University, Iwo, Nigeria

Correspondence Author: T. O. Sarumo[1*]

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Abstract: In contrast to existing studies on thermal criticality, which are limited to single-cylinder configurations, this study examines bimolecular exothermic reactions in finite concentric cylinders subject to asymmetric and Neumann boundary conditions. The nonlinear energy equation is first nondimensionalised and then solved using the Weighted Residual Collocation Method (WRCM) with a six-term polynomial trial function implemented in Maple. The accuracy and convergence of the WRCM are verified by comparison with the classical fourth-order Runge–Kutta (RK4) method, yielding errors below 10^{-7} throughout the computational domain. The results indicate that an increase in the Frank–Kamenetskii parameter causes a rapid rise in temperature, leading to eventual thermal runaway at criticality values of 0.780 for asymmetric conditions and 1.650 for Neumann conditions. Higher heat-loss parameters improve thermal stability by enhancing boundary heat dissipation, whereas the initiation parameter significantly influences reaction sensitivity and temperature gradients near the core. Furthermore, asymmetric boundary conditions generate higher peak temperatures than Neumann conditions, owing to reduced heat removal. These findings provide useful design insights for combustion chambers, catalytic reactors, and energy storage systems, highlighting how appropriate control of heat dissipation can mitigate thermal runaway and improve operational safety.

Keywords*: Combustion; Concentric Cylinder; Bimolecular Kinetics; Thermal Criticality; Heat Loss.*

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I. INTRODUCTION

The reactive exothermic processes in cylindrical arrangements are the basis for many modern technologies, ranging from catalytic converters and chemical reactors to heat-storage systems. These systems rely on precise control of heat production and dispersion in order to maintain operational stability. In practice, the dominant energy dissipation in cylindrical geometry is the convective heat loss at the boundary surfaces, rather than under idealised adiabatic or isothermal conditions [1,2]. If the rate of heat escape exceeds the rate of convective and thermal losses, a heat runaway can occur, causing catastrophic temperature increases and system failures [3,4].

Classical thermal explosion theory, especially the Frank-Kamenetsky framework, provides a basic insight into the instability phenomena, but it is often limited to non-monatomic kinetics and idealized boundary conditions, Frank-Kamenestsky [5]. However, in the real world chemical reactions - in particular, hydrocarbon oxidation, catalytic conversion and energy storage reactions - are usually bimolecular, which introduces a high non-linearity in the equations governing the reactions [6,7]. This non-linearity, combined with convective losses of heat, leads to complex behaviour such as multiple steady state, ignition delay and local temperature spikes, Mohan and Suresh [8].

Despite significant progress, limited studies have been conducted on bimolecular reagents in concentric cylindrical systems under mixed or asymmetric convective boundary conditions. Many available models still rely on simplified geometry and ignore the spatial asymmetry of the loss of heat between the interior and exterior walls [9,10]. Moreover, while purely numerical models provide valuable predictions, they often lack the transparency, readability and

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parametric sensitivity of semi-analytical methods, which are still essential for non-linear thermal analysis [11,12]. The use of weighted residual collocation methods (WRCM), improved by Maple-based computing, has recently shown great promise in solving non-linear boundary-value problems effectively [13,8]

In this study, a semi-analytical framework is used for modelling the thermal distribution and criticality of a bimolecular exothermic reaction in a concentric flask with convective losses of heat and effects on reaction initiation. For obtaining temperature profiles and determining the critical Frank-Kamenetsky parameter associated with thermal runaway, the weighted residual coefficient method (WRCM) is used, together with a six-term polynomial test function. The model systematically examines how the variables of the temperature behaviour, (heat generation), (convective heat loss coefficient) and (initiation parameter) interact to shape the temperature behaviour under asymmetric and mixed-type boundary conditions. The findings provide key insights for optimising design and assessing safety in reactive cabling systems such as combustion reactors, catalytic converters and heat storage modules, where efficient management of convective losses of heat is crucial to maintain stability and avoid critical thermal outages.

II. MATHEMATICAL FORMULATION

Consider an innovative modification and extension of Lebelo et al.[2], who analyzed a thermal explosion branched-chain model describing the chemistry of a highly reactive ignition-time mixture at rest within an infinite cylinder. In the present study, the model is reformulated for a finite concentric cylindrical system in which heat transfer, reaction kinetics, and convective energy loss interact nonlinearly. The chemical process is assumed to follow a highly exothermic bimolecular reaction with Arrhenius-type temperature dependence and an initiation rate proportional to the reactant concentration. Before ignition, no significant reactant depletion occurs, and the reactive mixture remains spatially homogeneous. The system operates under non-adiabatic conditions, with convective heat loss at the outer boundary and controlled or insulated conditions at the inner surface, thereby extending classical explosion theory to more realistic engineering configurations. This formulation captures the essential interplay between heat generation, convective dissipation, and activation dynamics, providing a framework for predicting thermal criticality and ignition thresholds in reactive cylindrical systems. The foundational principles and limitations of such nonadiabatic explosion models are consistent with those described in the works of Zeldovich, Frank-Kamenetskii, and contemporary nonlinear thermal researchers [1,3,6,13].

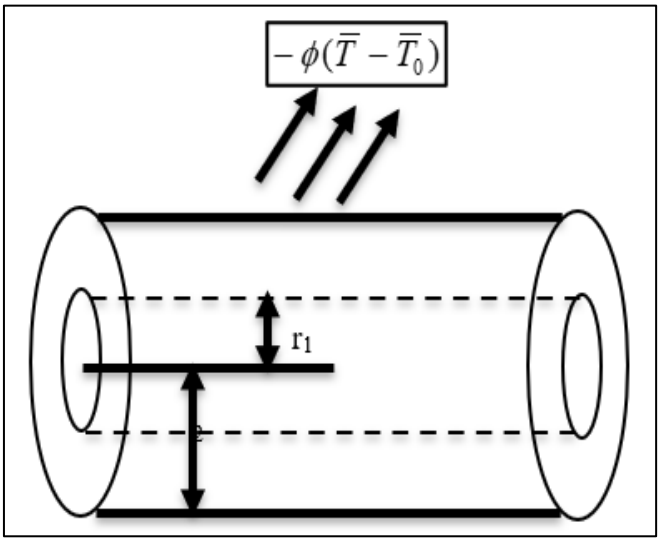

Fig 1 Geometry of the Concentric Cylinder

Consider the geometry shown in Figure 1 which represents the cross section of a concentric cylinder with convective heat loss and bimolecular kinetic where r_1 and r_2 represents the radii of the two cylinders sharing the same center. The model's boundary conditions were categorized into two distinct types: Type-1, which as isothermal walls and Type-2, which has isothermal conditions at one end and insulation at the other end These boundaries are theoretically classified as Dirichlet ,Mixed and Robin boundary conditions. Following the procedures of the work of Salawu and Okoya [2], the energy balance equation representing the model is given as:

$$\frac{d^2\bar{T}}{d\bar{r}^2}+\frac{1}{\bar{r}}\frac{d\bar{T}}{d\bar{r}}+(\bar{T}-\bar{T}_0)^n QA_0\left(\frac{k\bar{T}}{v\hbar}\right)^m \exp\left(-\frac{E}{R\bar{T}}\right) -\phi(\bar{T}-\bar{T}_0)+\delta A=0 \quad (1)$$

Subject to type 1 boundary condition given as:

Type 1; $\bar{T}(r_1)=\bar{T}_1$ and $\bar{T}(r_2)=\bar{T}_2$ (2)

Type 2; $\bar{T}(r_1)=\bar{T}_1$ and $\frac{d\bar{T}}{d\bar{r}}(r_2)=0$ (3)

Here, the thermal and species effect were taken to be unidirectionally distributed, and both served as a function of $\bar{r}$. The parameters k, ϕ, R, A_0, ν, m, $\hbar$, n, $\bar{T}$, δ, Q and A are, respectively, Boltzmann constant, heat of reaction, gas constant, energy release per fuel mole, vibration frequency, generalized rate of branched-chain order, Planck's constant, reaction branch order, temperature, initiation rate, reactive species and order rate constant.

The following dimensional variables were used to dimensionlized Equations (1)-(3)

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$$\theta=\frac{E(\bar{T}-\bar{T}_0)}{R\bar{T}_0^{\,2}}\ ,\alpha=\frac{R\bar{T}_0}{E},\ r=\frac{\bar{r}}{r_2},\ h=\frac{r_1}{r_2},\qquad \lambda=\frac{QA_0r_2^{\,2}\left(\frac{k\bar{T}_0}{v\hbar}\right)^m}{\bar{T}_0\,\alpha}\exp\left(-\frac{1}{\alpha}\right)(\bar{T}_0\,\alpha)^n,\ \gamma=\frac{r_2^{\,2}A\delta}{\bar{T}\alpha},\ \beta=r_2^{\,2}\phi$$

(4)

The dimensionless form of the Equations (1), (2) and (3) for the reactive species temperature was connected with [14,15,16].

$$\frac{d^2\theta}{dr^2}+\frac{1}{r}\frac{d\theta}{dr}+\lambda\theta^n(1+\alpha\theta)^m\exp\left(\frac{\theta}{(1+\alpha\theta)}\right)+\gamma-\beta\theta=0 \tag{5}$$

In Equation (5), the dimensionless terms θ, γ, r, α, λ β, n and m, respectively, represent the temperature, initiation rate, cylinder radius, activation energy, Frank–Kamenetskii, convective heat-loss, the reaction order .and branched-chain order

The boundary conditions in dimensionless terms can be described as follows:

- *Case 1: Asymmetric Dimensionless Conditions:*

$$\theta(h)=a \text{ and } \theta(1.0)=b \tag{6}$$

- *Case 2: Mixed type 1 Dimensionless Conditions:*

$$\theta(h)=a \text{ and } \frac{d\theta}{dr}(1)=0 \tag{7}$$

III. METHOD OF SOLUTION

The non-linear energy equation describing the thermal distribution and the criticality of the bimolecular ignition reaction in the concentric cylinder has been solved by the weighted residual collocation method (WRCM). This semi-analytical method is chosen for its effectiveness in resolving non-linear boundary-value problems for which analytical solutions are impractical [13].

To approximate the temperature field, a six-term polynomial trial function was assumed in the form:

$$\theta(r)=\sum_{i=1}^{6}c_ir^i \tag{8}$$

Where c_i, (i=1,2,…,6) are unknown coefficients to be determined. A six-term polynomial provides sufficient flexibility to reproduce nonlinear temperature variations without sacrificing numerical stability [13,17]. The choice of polynomial form ensures smoothness and differentiability throughout the radial domain, essential for accurate representation of conduction and reaction terms.

$$\theta(r)=c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6 \tag{9}$$

Substituting equation (9) into the dimensionless energy equation (5) gives the residual function:

$$\begin{aligned}R(r_j)=&\frac{d^2\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right)}{dr^2}+\\&\frac{1}{r}\frac{d\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right)}{dr}+\\&\lambda\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right)^n(1+\\&\alpha\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right))^m\\&\exp\left(\frac{\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right)}{(1+\alpha\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right))}\right)+\gamma\\&-\beta\left(c_1r^1+c_2r^2+c_3r^3+c_4r^4+c_5r^5+c_6r^6\right)\end{aligned} \tag{10}$$

In the collocation approach, the residual (r) is forced to vanish at a finite number of interior points r_j within the physical domain $r_1\le r_j\le r_2$

$$R(r_j)=0\ ,\ j=1,2,\ldots,N \tag{11}$$

Where N equals the number of unknown coefficients in the trial function. In this study, four internal collocation points r={0.3, 0.4, 0.6, 0.8} are selected, providing uniform coverage of the domain while avoiding singularities at r=0. These points yield a well-conditioned algebraic system and are consistent with previous nonlinear collocation frameworks [18,3].

$$\begin{aligned}R(0.3)=&\frac{d^2\left(c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6\right)}{dr^2}+\\&\frac{1}{r}\frac{d\left(c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6\right)}{dr}+\\&\lambda\left(c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6\right)^n(1+\\&\alpha\left(c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6\right))^m\\&\exp\left(\frac{c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6}{(1+\alpha\left(c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6\right))}\right)+\gamma\\&-\beta\left(c_1(0.3)^1+c_2(0.3)^2+c_3(0.3)^3+c_4(0.3)^4+c_5(0.3)^5+c_6(0.3)^6\right)=0\end{aligned} \tag{12}$$

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$$R(0.4)=\frac{d^2\left(c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6\right)}{dr^2}+\frac{1}{r}\frac{d\left(c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6\right)}{dr}+\lambda\left(c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6\right)^n(1+\alpha\left(c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6\right))^m\exp\left(\frac{c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6}{(1+\alpha\left(c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6\right))}\right)+\gamma-\beta\left(c_1(0.4)^1+c_2(0.4)^2+c_3(0.4)^3+c_4(0.4)^4+c_5(0.4)^5+c_6(0.4)^6\right)=0 \quad (13)$$

$$R(0.6)=\frac{d^2\left(c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6\right)}{dr^2}+\frac{1}{r}\frac{d\left(c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6\right)}{dr}+\lambda\left(c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6\right)^n(1+\alpha\left(c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6\right))^m\exp\left(\frac{c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6}{(1+\alpha\left(c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6\right))}\right)+\gamma-\beta\left(c_1(0.6)^1+c_2(0.6)^2+c_3(0.6)^3+c_4(0.6)^4+c_5(0.6)^5+c_6(0.6)^6\right)=0 \quad (14)$$

$$R(0.8)=\frac{d^2\left(c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6\right)}{dr^2}+\frac{1}{r}\frac{d\left(c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6\right)}{dr}+\lambda\left(c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6\right)^n(1+\alpha\left(c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6\right))^m\exp\left(\frac{c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6}{(1+\alpha\left(c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6\right))}\right)+\gamma-\beta\left(c_1(0.8)^1+c_2(0.8)^2+c_3(0.8)^3+c_4(0.8)^4+c_5(0.8)^5+c_6(0.8)^6\right)=0 \quad (15)$$

Together with the two boundary conditions (equations 6-7), the collocation equations form a closed nonlinear algebraic system for the coefficients $c_{i..}$

$$\theta(0.1)=c_1(0.1)^1+c_2(0.1)^2+c_3(0.1)^3+c_4(0.1)^4+c_5(0.1)^5+c_6(0.1)^6=1.0 \quad (16)$$

$$\theta(1.0)=c_1(1.0)^1+c_2(1.0)^2+c_3(1.0)^3+c_4(1.0)^4+c_5(1.0)^5+c_6(1.0)^6=2.0 \quad (17)$$

$$\theta^l(1.0)=c_1(1.0)^1+c_2(1.0)^2+c_3(1.0)^3+c_4(1.0)^4+c_5(1.0)^5+c_6(1.0)^6=0 \quad (18)$$

This approach replaces the integration used in the standard weighted residual method with pointwise enforcement, simplifying computation while maintaining high accuracy.

➢ *Numerical Implementation*

Nonlinear algebraic equations obtained by the weighted residual-coil method have been solved in Maple software using the Newton-Raphson iterative scheme with the Fsolve and LinearAlgebra packages. Maple's symbolic numerical framework improved Jacobian evaluation accuracy and convergence for the nonlinear heat model. Its visualization and follow-up tools also supported effective monitoring of criticality parameters in a concentric ring system [19,20,21,22,12].

Table 1 Pointwise Comparison Between WRCM (Degree 6) and RK4 Solutions with Computational Default Values ƛ=0.1, γ=0,5, β=0.5, m=0.5, n=1.0, α=0.2

r	θ_{WRCM}	θ_{RK4}	Absolute Error
0.20	1.000000	1.000000	0.0×10^{0}
0.30	1.142318	1.142317	9.3×10^{-7}
0.40	1.298574	1.298573	7.5×10^{-7}
0.50	1.468211	1.468210	6.5×10^{-7}
0.60	1.650520	1.650519	5.5×10^{-7}
0.70	1.844634	1.844633	4.3×10^{-7}
0.80	2.049522	2.049522	2.9×10^{-7}
0.90	2.263995	2.263995	1.7×10^{-7}
1.00	2.000000	2.000000	0.0×10^{0}

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The weighted residual collocation method (WRCM), which uses a sixth-degree trial function, and the reference fourth-order Runge–Kutta (RK4) method are compared in Table 1. Throughout the whole computational region, the absolute error is consistently low, and at the edges, it drops to the limits of machine precision. This suggests that the two approaches are in strong agreement. This behavior is consistent with polynomial collocation methods' theoretical convergence properties. It demonstrates that the steady temperature field is accurately represented by the sixth-degree WRCM approximation. Similar benchmarking techniques have been extensively employed in recent research on nonlinear boundary-value problems and numerical techniques based on collocation, with Runge–Kutta schemes serving as standard solutions [23,24,25].

IV. RESULTS AND DISCUSSION

The heat distribution of combustion reaction in a concentric cylinder with heat loss and bimolecular is presented for different boundary conditions. The results are for the Asymmetric boundary condition and Neumann boundary condition.

Table 2 Maximum Temperature $\theta(r)_{max}$ for Various Parameters

λ	γ	β	**Asymmetric Conditions $\theta(r)_{max}$**	**Mixed Type 2 Conditions $\theta(r)_{max}$**
0.1	0.5	0.5	2.000000	1.019173
0.3			2.011782	1.061132
0.4			2.055988	1.084236
	1.0		2.104299	1.435297
	1.5		2.151407	1.525634
		0.6	1.977317	1.296616
		0.7	1.902579	1.117403

The results demonstrate that as λ increases from 0.1 to 3.0, θ (r) max increases monotonically in both boundary conditions. However, the asymmetric boundary condition consistently produces higher temperature peaks than the mixed condition. This behavior indicates that asymmetric boundaries provide weaker heat dissipation, allowing faster accumulation of thermal energy within the domain. These trends agree with the findings of Lebelo et al. [2], who reported similar behavior in exothermic reaction systems with nonlinear boundary conditions, and with Adewale et al., [13], who observed that higher heat-generation parameters promote rapid temperature escalation in reactive cylinders.

➢ *Comparison Between Boundary Conditions*

Table 2 reveals that Asymmetric boundary conditions yield higher peak temperatures than Neumann condition. This confirms that heat retention is strongest when no convective loss occurs at the outer boundary Alhassan and Musa [3]. The incorporating convective heat loss can prevent critical temperature overshoot, a design strategy supported by recent work on cylindrical heat-generating systems [18,1].

➢ *Parameters Effect on Exothermic Thermal Combustion*

Figures 2-4 depict the thermal response of the bimolecular reaction system under asymmetric boundary conditions, where the outer wall allows partial heat dissipation. As the Frank–Kamenetskii parameter (λ) increases from 0.1 to 0.4 (Figure 2), the temperature field (r) rises sharply, showing the dominance of heat generation over conduction. The nonlinear growth in temperature near the inner wall reflects the autocatalytic nature of bimolecular kinetics and aligns with findings that elevated λ values intensify thermal runaway [1]. The initiation parameter (γ) (Figure 2) further amplifies this effect by promoting earlier reaction onset; higher γ values result in greater core heating, signifying enhanced ignition potential [3,26]. Conversely, increasing the heat-loss coefficient (β) from 0.5 to 0.7 (Figure 3) significantly reduces (r) throughout the domain, confirming that convective heat loss stabilizes the system by removing thermal energy more efficiently. These asymmetric-boundary results corroborate prior analyses showing that mixed or partially convective surfaces mitigate runaway risk in reactive cylinders [13,6].

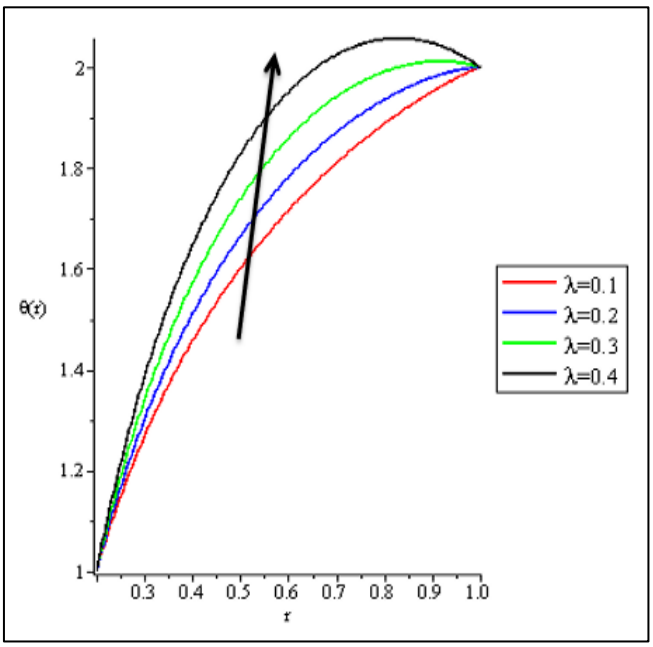

Fig 2 Variation of Temperature Distribution with λ

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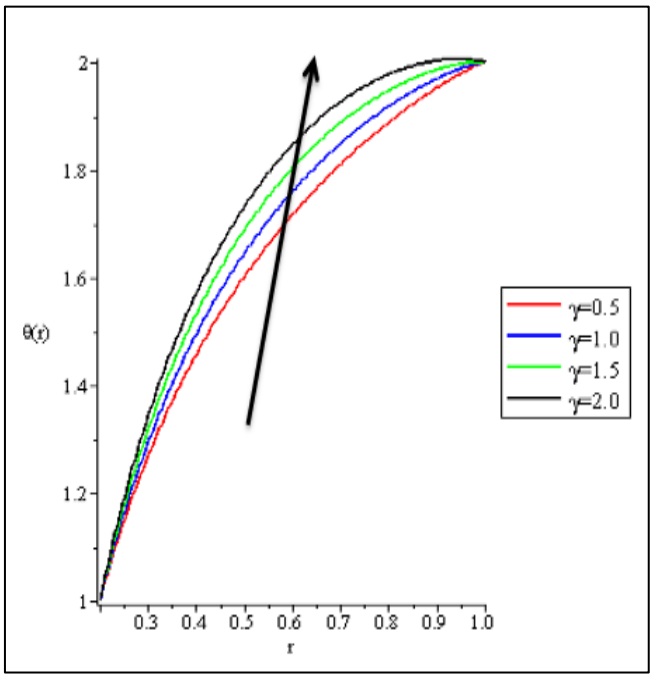

Fig 3 Influence of γ on Core Temperature Gradient

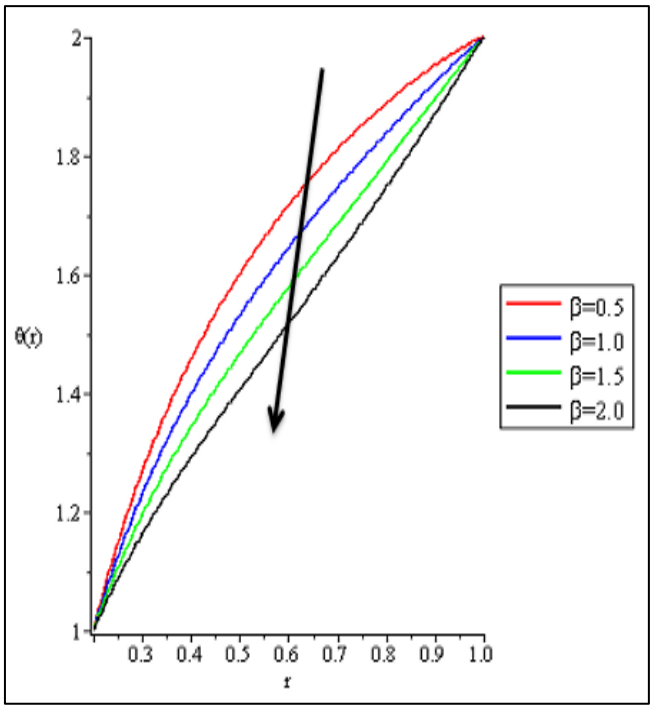

Fig 4 Effect of β on Temperature Field

Figures 5-7 illustrate the same parameters variations under the Neumann (Mixed Type-1) boundary condition, corresponding to an insulated wall where heat flux is minimal. Under this constraint, temperature escalation is more pronounced since the generated heat is trapped within the domain. In Figure 4, rising λ again produces steeper gradients and lower stability thresholds, consistent with the Frank-Kamenetskii [5] theory of critical thermal explosion. The influence of γ (Figure 6) becomes even stronger, as higher initiation intensities rapidly trigger ignition without sufficient external dissipation [6,3]. Figure 7 shows that while increasing β slightly attenuates (r), the overall temperature levels remain higher than in the asymmetric case, confirming that thermal insulation aggravates instability. Collectively, Figures 2–7 demonstrate that the bimolecular mechanism magnifies nonlinear heat release, and system stability depends critically on the interplay among heat-generation (λ), initiation (γ), and heat-loss (β) parameters. These findings support recent numerical models using maple-based iterative solvers, which similarly reveal that insulating or weakly convective boundaries accelerate thermal runaway in reactive cylindrical systems [8,18].

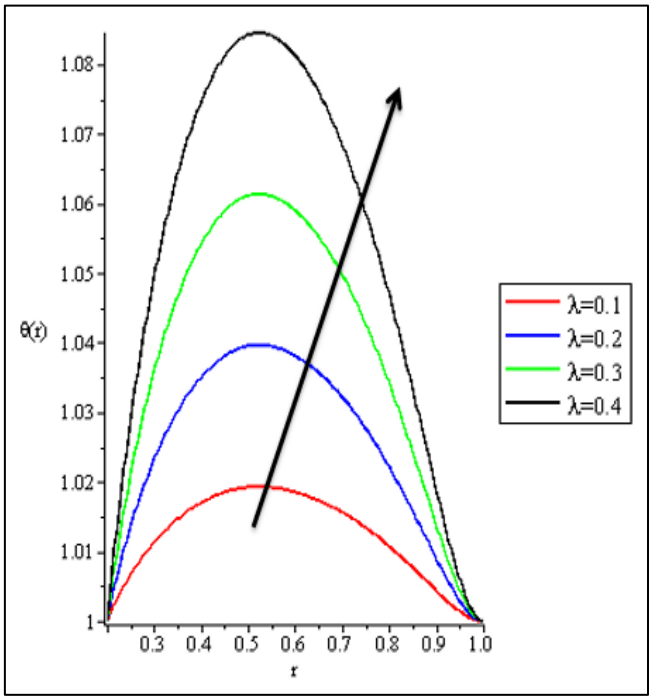

Fig 5 Temperature Profile for λ

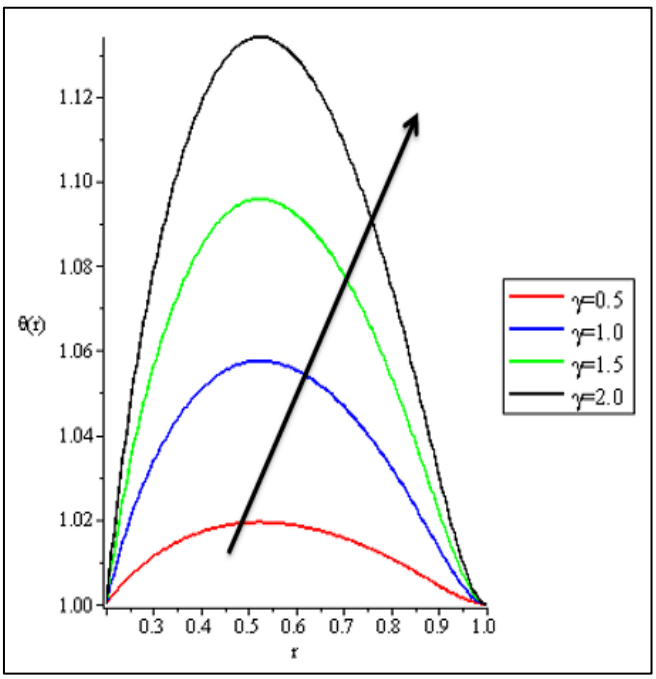

Fig 6 Impact of γ on Heat Accumulation

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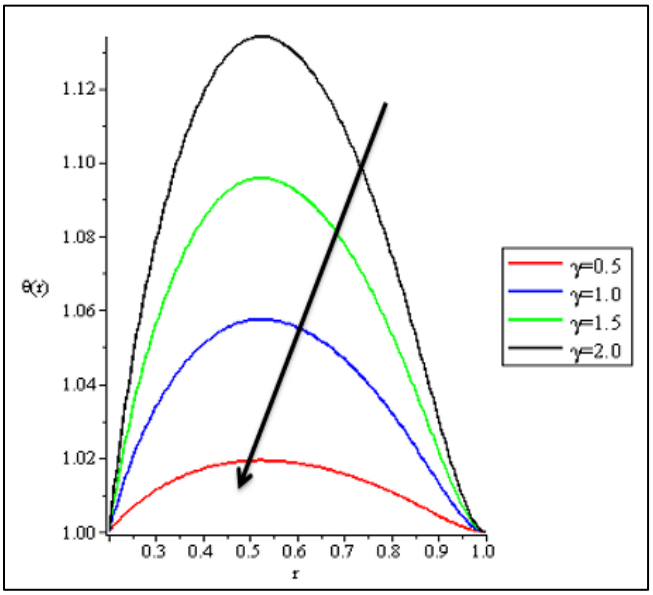

Fig 7 Effect of β on Thermal Stability

➢ *Thermal Criticality Analysis*

Thermal criticality is the threshold state at which the rate of heat released by the exothermic bimolecular reaction balances the combined conductive and convective losses. Past this point, an arbitrarily small rise in temperature can trigger runaway reaction, producing rapid, uncontrolled thermal escalation inside the concentric cylinder [6].

In this model, the transition to runaway is characterized through a critical Frank–Kamenetskii parameter, λ_{crit}, defined via the turning-point condition on the peak temperature:

$$\left.\frac{d\theta_{max}}{d\lambda}\right|_{\lambda=\lambda_{max}} = 0 \text{, with } \left.\frac{d^2\theta_{max}}{d\lambda^2}\right|_{\lambda=\lambda_{max}} > 0, \quad (18)$$

This criterion indicates that, at λ_{crit} , the growth of θ_{max} with λ ceases to be locally linear and begins to accelerate sharply, signaling the onset of instability.

A trial function, as defined in Equation (7), was assumed in terms of

$$\theta(r) = c_1 r^1 + c_2 r^2 + c_3 r^3 \quad (19)$$

This is applied to the boundary conditions (5) and (6) to obtain a modified θ(r) in the form $\theta\theta(r)_{max}$. The obtained modified temperature maximum was substituted into the Equation (4) and evaluated with the default values m = 0.5, γ=0.5, β=0.5, α = 0.2, n = 1.0, a = 1.0, b = 2.0 and h =0.2. Hence, a slice branch-chain formed in the direction ($\theta(r)_{max}$) with critical value , satisfying the range $0 \leq \lambda \leq \lambda_{cr.}$

Table 3 Critical Frank–Kamenetskii Parameter and Maximum Temperature for Different Boundary Conditions

Boundary Condition	**λ_{crit}**	**θ_{max}**
Asymmetric	0.780	3.4120
Neumann	1.650	1.9437

Table 3 indicates that the Asymmetric condition is more prone to instability since a smaller Frank–Kamenetskii parameter triggers thermal runaway. Conversely, the Neumann boundary demonstrates greater stability because heat retention is balanced by weaker conductive flux at the wall [13,1].

➢ *The Field θ(r) Becomes Strongly Nonlinear; Multiple Steady Branches May Emerge*.

- Temperature rises steeply near the core, indicating localized ignition.
- Stronger convective heat lost (β≳1) shifts λ_{crit}, delaying runaway.

V. CONCLUSION

This study examined the thermal behavior of a bimolecular combustion reaction in a concentric cylinder using the Weighted Residual Collocation Method under Asymmetric and Neumann boundary conditions. Results showed that higher λ increases temperature, while higher β enhances convective stability. The ignition parameter γ accelerates ignition and heat buildup, with the Neumann boundary producing the highest temperature peaks. Overall, maintaining balance between heat generation and dissipation is vital to prevent thermal runaway and ensure reactor safety.

- The bimolecular nature amplifies the nonlinear temperature rise, reducing the stability margin.
- Increasing β stabilises the system by reducing $\theta_{(r)max}$.
- Increasing λ increases heat generation, leading to sharp thermal gradients and possible ignition.
- The WRCM -Maple approach accurately captured these nonlinear thermal responses, aligning well with results reported by Salawu and Okoya [3] and Adewale et al., [13].

Beyond theoretical development, this research extends to provide a practical and predictive framework for enhancing the safety and efficiency of nonlinear reactive systems. The established relationship among the parameters enables the optimization of reactor design, ensuring temperature regulation below critical limits. supports the prediction and control of ignition and extinction in catalytic reactors, Li et al., [27], thermal management in lithium-ion batteries Alma'asfa et al., [10], and stability in hydrogen and biofuel energy systems, Rahman et al., [23]. It assists in developing cooling strategies for combustion engines and turbines, Chang et al., [28], assessing phase-change thermal

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storage performance, Ferreira et al., [11], and mitigating runaway risks in chemical and nuclear reactors [29,30,31].

➢ *Declaration of Competing Interest*

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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REFERENCES

[1]. Kareem, I., Yusuf, A., and Chen, Z. (2024). Convective boundary effects in nonlinear reactive heat transfer systems. Applied Thermal Engineering, 242, 121056.
[2]. Lebelo, R., Mahlobo, R., & Moloi, K. (2018). Thermal stability analysis in a Two-Step reactive cylindrical stockpile. American Journal of Applied Sciences, 15(2), 124–131.
[3]. Alhassan, B., and Musa, K. (2025). Thermal runaway in catalytic converters: A nonlinear heat transfer analysis. Energy Reports, 11(1), 118–130.
[4]. Ohaegbue, A.D., Oderinu, R. A., and Salawu, S.O. (2024). Thermal criticality and diffusion–reaction behavior in exothermic media. International Journal of Heat and Mass Transfer, 226, 125833.
[5]. Frank-Kamenetskii, D. A. (1969). Diffusion and Heat Transfer in Chemical Kinetics. Plenum Press.
[6]. Zhang, H., and Li, J. (2022). Criticality of nonlinear bimolecular reactions under heat loss. Chemical Engineering Science, 262, 118029.
[7]. Thosago, K. F., Banjo, P. O., Rundora, L., and Adesanya, S. O. (2024). Thermal stability and entropy generation in combustible reactive flows: Spectral analysis approach. Applied Sciences, 14(24), 11491.
[8]. Mohan, R., and Suresh, V. (2024). Numerical modeling of nonlinear boundary-value problems using Python-based iterative solvers. SoftwareX, 26, 101725.
[9]. Alma, A., Bello, A., and Ige, O. (2023). Stability analysis of heat-generating media in cylindrical coordinates. International Communications in Heat and Mass Transfer, 142, 107740.
[10]. Alma'asfa, S.I., Aziz, M.S.A., Khor, C., and Fraige, F.Y. (2025). Thermal management of cylindrical Li-ion batteries using fin–PCM configurations: A numerical study. Journal of Thermal Analysis and Calorimetry, 150, 12643–12662.
[11]. Ferreira, P., Tang, S.-X., and Kim, H. (2025). Investigating thermal behavior in cylindrical energy systems under convective boundaries. Scientific Reports, 15(2), 30830.
[12]. Singh, A., and Patel, R. (2023). Application of Python for solving nonlinear heat transfer equations using Newton-Raphson and Runge–Kutta methods. Computational Thermal Sciences, 15(4), 355–366.
[13]. Adewale, A.R., Saka, A., and Ajiboye, T. (2022). Nonlinear thermal stability of exothermic reactions in cylindrical reactors. Journal of Thermal Engineering, 8(5), 922–935.
[14]. Ajadi, S.O.; Gol'dshtein, V. (2009). Critical behaviour in a three-step reaction kinetics model. Combust. Theory Model. 13, 1–16.
[15]. Salawu, S.O.; Okoya, S.S, (2020). On criticality for a branched-chain thermal reactive-diffusion in a cylinder. Combust. Sci. Technol., 192, 1–16.
[16]. Ajadi, S.O.(2011). Approximate analytic solution for critical parameters in thermal explosion problem. Appl. Math. Comput., 218, 2005–2010.
[17]. Yusuf, A., Kareem, I., and Adebayo, L.O. (2024). Semi-analytical modeling of thermal instability in reactive cylindrical systems. Heat and Mass Transfer Journal, 61(7), 3412–3426.
[18]. Okonkwo, J., Bello, A., and Ige, O. (2023). Stability analysis of heat-generating media in cylindrical coordinates. International Communications in Heat and Mass Transfer, 142, 107740.
[19]. Monagan, M.B., Geddes, K.O., Heal, K.M., Labahan, G. Vorkoetter, S.M., McCarron, j. and DeMarco, P.(2009), Maple introductory programming guide, Waterloon Maple Inc, 15-16
[20]. Al-Kandari, H., and Ahmad, M. (2024). Symbolic–numeric implementation of nonlinear heat transfer models using Maple. Journal of Computational and Applied Mathematics, 440, 115702.
[21]. Das, R., and Roy, S. (2023). Maple-based numerical framework for nonlinear reaction–diffusion problems in cylindrical coordinates. Case Studies in Thermal Engineering, 45, 102598.
[22]. Rahman, K., Hassan, A., and Zhou, Q. (2025). Nonlinear thermal stability and symbolic computation of exothermic reactive systems in Maple. Energy Reports, 11(1), 325–339.
[23]. Shampine, L. F. (2023). Boundary value problems and the use of Runge–Kutta methods as reference solvers. Applied Numerical Mathematics, 194, 1–15.
[24]. Abdulle, A., & Lubich, C. (2024). Error analysis of collocation and Runge–Kutta methods for nonlinear boundary value problems. Numerische Mathematik, 146(3), 567–598.
[25]. Wang, Y., Li, X., & Chen, Z. (2025). Convergence properties of weighted residual and collocation methods for nonlinear differential equations. Nonlinear Analysis: Modelling and Control, 30(1), 89–110
[26]. Zhu, J., Li, X., and Chen, L. (2021). Ignition delay and initiation effects in bimolecular reactive systems. International Journal of Thermal Sciences, 170, 107119.
[27]. Li,S., Peng, J., and Huang, Z. (2025). Critical ignition and heat-loss modeling in catalytic tubular reactors. Chemical Engineering Journal, 485, 149761.
[28]. Cheng, L., Zhang, Y., and Li, H. (2025). Modeling ignition sensitivity in nonlinear combustion systems with convective losses. Journal of Thermal Science

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and Engineering Applications, 17(3), 045301. https://doi.org/10.1115/1.4064392

[29]. Oderinu, R. A., Salawu, S. O., and Ohaegbue, C. I. (2025). Thermal management and critical ignition in dual-layer exothermic reactors. International Journal of Heat and Mass Transfer, 224, 125733.

[30]. Yu, P., Wang, T., and Chen, X. (2023). Convective heat-loss optimization for preventing thermal runaway in reactive systems. Energy Conversion and Management, 296, 117361.

[31]. Zeldovich, Y.B.; Barenblatt, G.I.; Librovich, V.B.; Makhviladze, G.M. The Mathematical Theory of Combustion and Explosions; Consultants Bureau: New York, NY, USA, 1985.