Temperature oxidation of double combustible reaction and thermal ignition in a concentric cylinder with diverse boundary constraints

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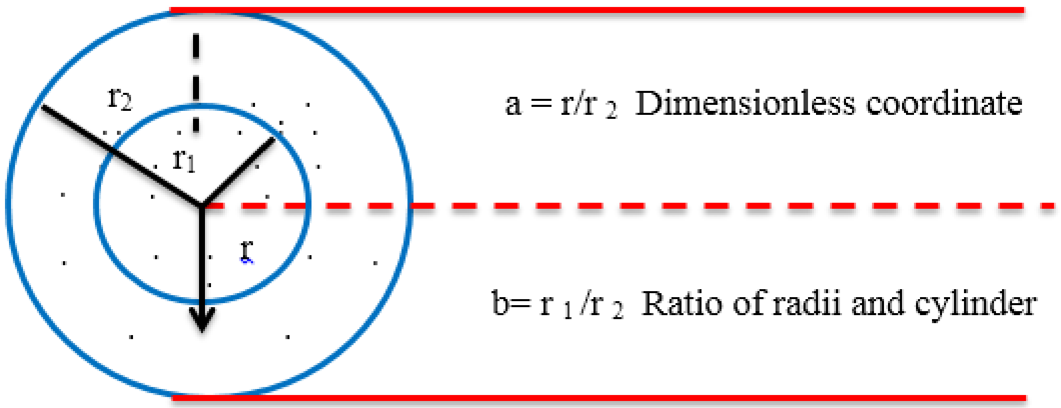
Abstract

Chemical species undergoing spontaneous reactions and temperature oxidation of materials are useful in explosion safety, propulsion detonation and chemical synthesis. Thus, this study considers the dynamics of temperature oxidation of a two-step exothermic combustion and thermal ignition in a concentric isothermal cylinder with diverse boundary constraints. With constant thermal reactant conductivity and diffusion, a time-dependent partial derivative model is developed to give insight into the chemistry of the branch chain reaction, pre-exponential factor, Arrhenius kinetic, and critical behaviour of the system. A finite semi-discretization difference method provides a numerical solution to the model. An investigation is carried out on the various boundary conditions impact on the thermal distribution, stability and ignition of the homogenous species reactant.

Model Assumptions

Consider the chemistry of the branch-chain explosion model for reactant diffusion at rest without pre-mixture of combustible species in an indefinite concentric cylinder. An exothermic irreversible reaction occurs in a device subject to asymmetric constraints, mixed type-one constraints, and mixed type-two constraints with Arrhenius exponential approximate and activation energy.



Mathematical Equation

$$\rho Cp\frac{\partial\phi}{\partial\bar{t}} = k\frac{1}{\bar{r}}\frac{\partial}{\partial\bar{t}}\left(\bar{r}\frac{\partial\phi}{\partial\bar{t}}\right) - \alpha(\phi-\phi_w) + A_1C_1Q_1\left(\frac{K\phi}{\upsilon a}\right)^n \exp\left(-\frac{E_1}{R\phi}\right) + A_2C_2Q_2\left(\frac{K\phi}{\upsilon a}\right)^n \exp\left(-\frac{E_2}{R\phi}\right), \tag{4}$$

the corresponding initial constraints is:

$$\phi(\bar{r},0) = \phi_0, \tag{5}$$

the applicable different concentric cylinder boundary constraints are given as Okoya [], Salawu and Okoya []:

$$\begin{aligned}&\text{Case A: Asymmetric constraints } \phi(r_1,\bar{t}) = \phi_1 \text{ and } \phi(r_2,\bar{t}) = \phi_2,\\ &\text{Case B: Mixed type-I constraints } \phi(r_1,\bar{t}) = \phi_1 \text{ and } \frac{\partial\phi}{\partial\bar{r}}(r_2,\bar{t}) = 0,\\ &\text{Case C: Mixed type-II constraints } \frac{\partial\phi}{\partial\bar{r}}(r_1,\bar{t}) = 0 \text{ and } \frac{\partial\phi}{\partial\bar{r}}(r_2,\bar{t}) + B\phi(r_2,\bar{t}).\end{aligned} \tag{6}$$

Model Transformation

$$t = \frac{k\bar{t}}{c^2\rho Cp}, c = \frac{r_1}{r_2}, r = \frac{\bar{r}}{r_2}, \vartheta = \frac{E_1(\phi - \phi_w)}{R\phi_w^2}, \vartheta_0 = \frac{E_1(\phi_0 - \phi_w)}{R\phi_w^2}, \delta = \frac{R\phi_w}{E_1}, m = \frac{E_2}{E_1},$$
$$\beta = \left(\frac{K\phi_w}{\upsilon a}\right)^n \frac{A_1 C_1 Q_1 E_1 c^2}{kR\phi_w^2} \exp\left(-\frac{E_1}{R\phi}\right), \chi = \frac{\alpha c^2}{k}, \lambda = \frac{A_2 E_2 Q_2}{A_1 E_1 Q_1} \exp\left(\frac{E_1 - E_2}{R\phi}\right), \tag{7}$$
$$\xi = \frac{\phi_1 - \phi_w}{R\phi_w^2}, \zeta = \frac{\phi_2 - \phi_w}{R\phi_w^2}, Bi = \frac{Br_2}{k}.$$

Utilizing equation (7) on equation (4) along with the initial and boundary constraints (5) and (6), the invariant dimensionless model is obtained as:

$$\frac{\partial\vartheta}{\partial t} = \frac{\partial^2\vartheta}{\partial r^2} + \frac{1}{r}\frac{\partial\vartheta}{\partial r} + \beta(1+\delta\vartheta)^n \exp\left(\frac{\vartheta}{1+\delta\vartheta}\right) + \beta\lambda(1+\delta\vartheta)^n \exp\left(\frac{m\vartheta}{1+\delta\vartheta}\right) - \chi\vartheta, \tag{8}$$

the initial constraint gives:

$$\vartheta(r, 0) = \vartheta_0, \tag{9}$$

the corresponding boundary constraints resulted to:

$$\begin{aligned}
&\text{Case A: Asymmetric constraints } \vartheta(c,t) = \xi \text{ and } \vartheta(1,t) = \zeta,\\
&\text{Case B: Mixed type-I constraints } \vartheta(c,t) = \xi \text{ and } \frac{\partial\vartheta}{\partial r}(1,t) = 0,\\
&\text{Case C: Mixed type-II constraints } \frac{\partial\vartheta}{\partial r}(c,t) = 0 \text{ and } \frac{\partial\vartheta}{\partial r}(1,t) + Bi\vartheta(1,t) = 0.
\end{aligned} \tag{10}$$

Numerical Solution

The boundary value partial derivative quasilinear model (8) to (10) is solved via a finite difference semi-discretization line method as demonstrated by [Burden and Douglas-Faires, Salawu and Okoya]. A h parts spatial range $0 \leq r_r \leq 1$ partition is done to allow grid points $r_i = \Delta(i-1)$, $1 \leq i \leq h+1$ and a grid size $\Delta r = 1/h$. A time space t is assumed, where $0 \leq j \leq N$, and N=1,2,3,.... Approximation of the second-order central finite differences $(O(N^2))$ is carried out for the spatial and time derivatives of the equations (8) to (10). Hence, the discretization of the two-step combustion model becomes

$$\begin{aligned}\frac{\vartheta_i^{j+1}-\vartheta_i^j}{\Delta t} &= \frac{1}{\Delta r^2}\left(\vartheta_{i+1}^j - 2\vartheta_i^j + \vartheta_{i-1}^j\right) + \beta\left(1+\delta\vartheta_i^j\right)^n \exp\left(\frac{m\vartheta_i^j}{1+\delta\vartheta_i^j}\right) - \chi\vartheta_i^j + \\ &\frac{1}{2r_i\Delta r}\left(\vartheta_{i+1}^j - \vartheta_{i-1}^j\right) + \beta\lambda\left(1+\delta\vartheta_i^j\right)^n \exp\left(\frac{m\vartheta_i^j}{1+\delta\vartheta_i^j}\right),\end{aligned} \tag{12}$$

the initial constraint gives

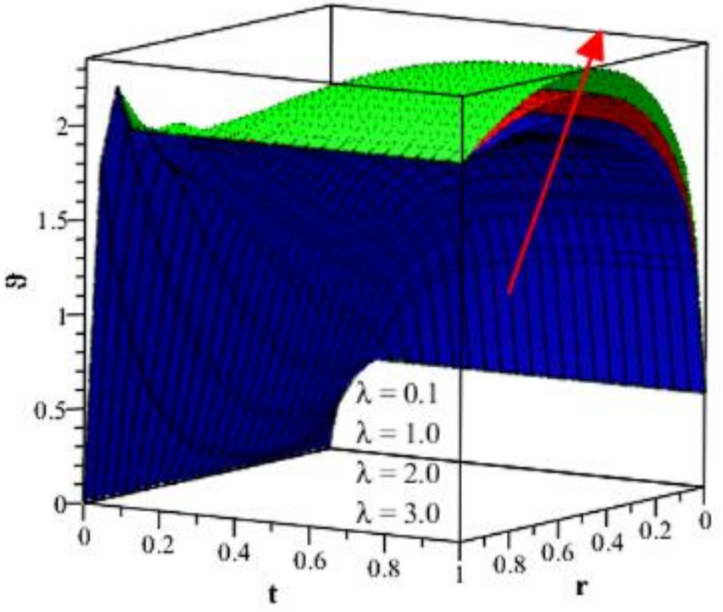
$$\vartheta_i = \vartheta_0, 1 \leq i \leq h+1. \tag{13}$$

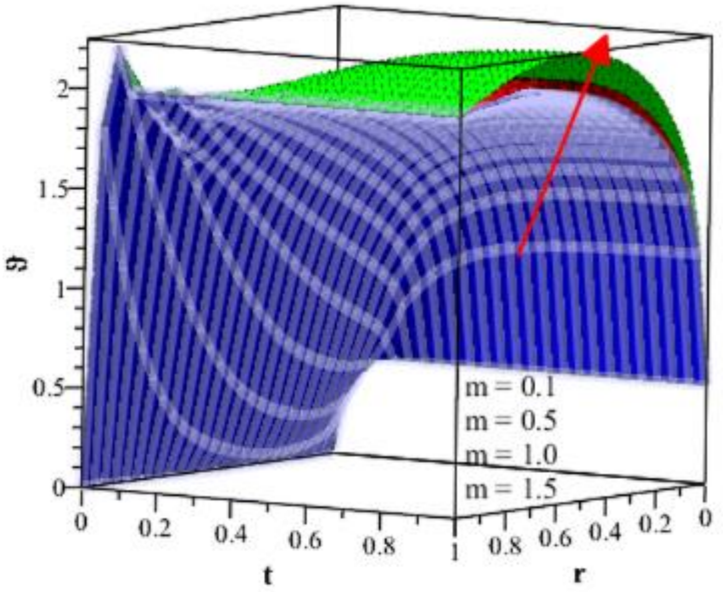
the boundary constraints are describe as:

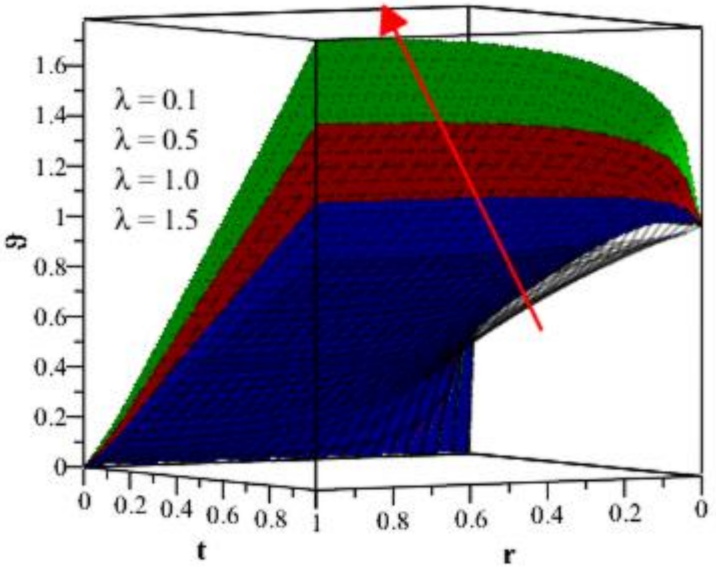
$$\begin{aligned}&\text{Case A: Asymmetric constraints } \vartheta_i = \xi \text{ and } \vartheta_{h+1} = \zeta,\\ &\text{Case B: Mixed type-I constraints } \vartheta_i = \xi \text{ and } \vartheta'_{h+1} = 0,\\ &\text{Case C: Mixed type-II constraints } \vartheta'_i = 0 \text{ and } \vartheta'_{h+1} + Bi\,\vartheta_{h+1} = 0.\end{aligned} \tag{14}$$

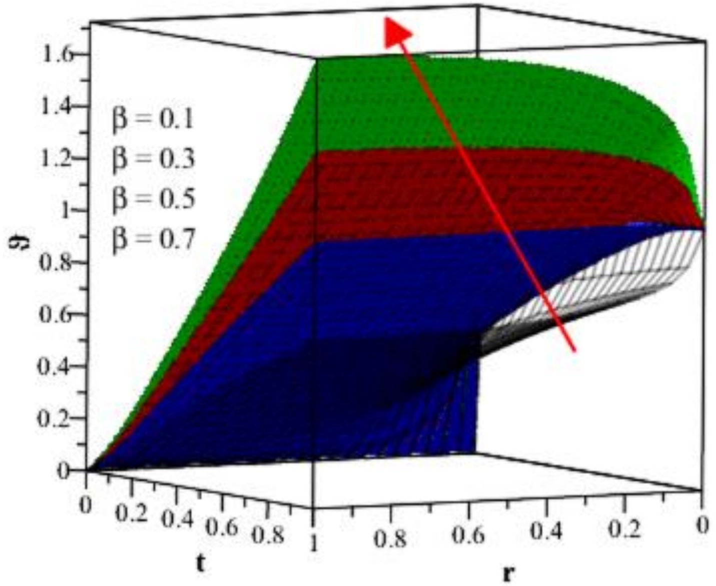
A Maple solver with an embedded finite difference method is used to computationally solve the model, and the solution outcomes are graphically expressed.

Results and Discussion

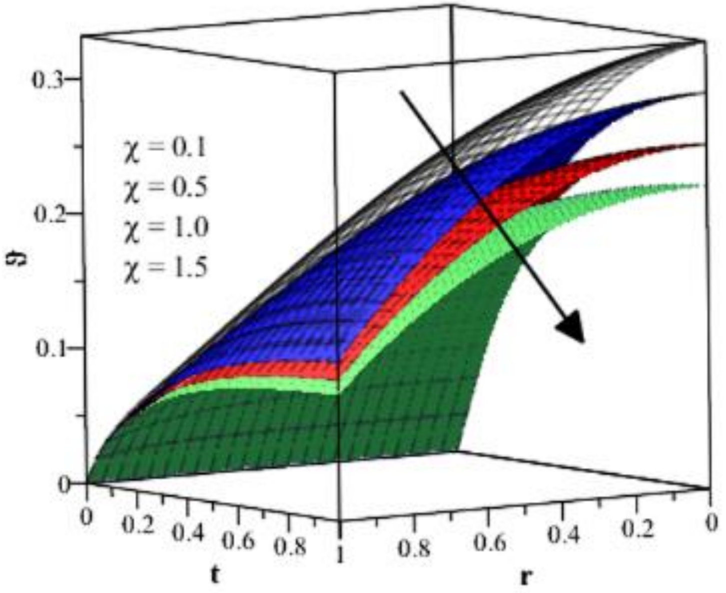


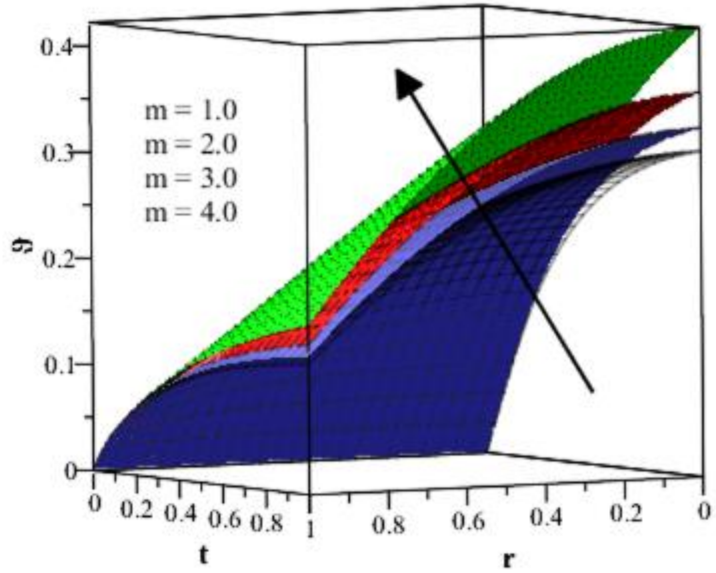


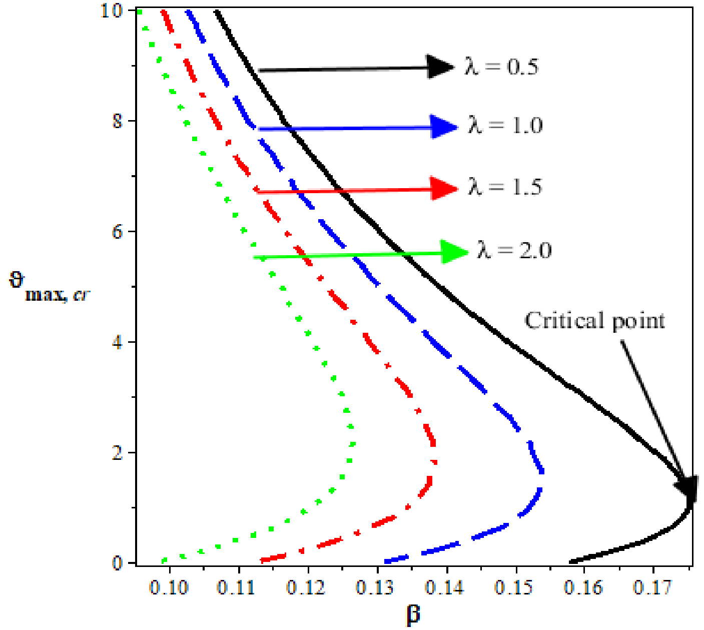


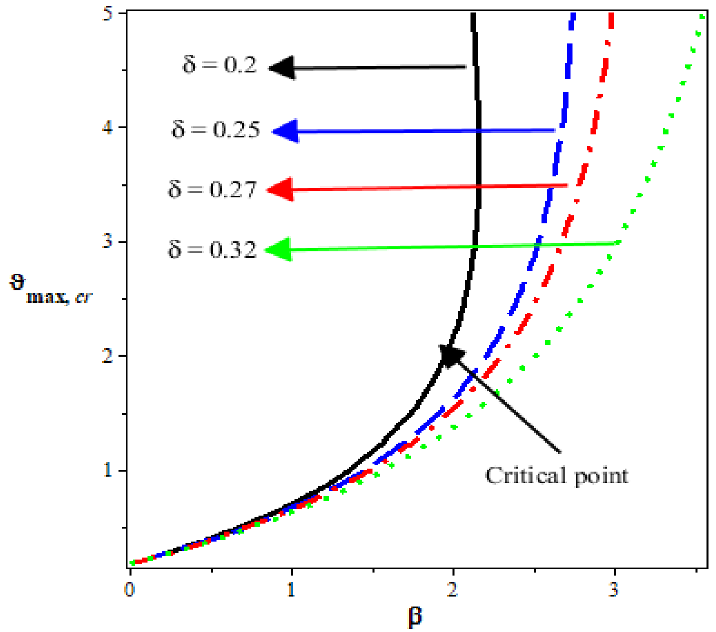


Results and Discussion Contd









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