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Research Article

Computational Modelling of Thermal Stability in a Reactive Slab with Reactant Consumption

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This paper investigates both the transient and the steady state of a one-step nth-order oxidation exothermic reaction in a slab of combustible material with an insulated lower surface and an isothermal upper surface, taking into consideration reactant consumption. The nonlinear partial differential equation governing the transient reaction-diffusion problem is solved numerically using a semidiscretization finite difference technique. The steady-state problem is solved using a perturbation technique together with a special type of the Hermite-Padé approximants. Graphical results are presented and discussed quantitatively with respect to various embedded parameters controlling the systems. The crucial roles played by the boundary conditions in determining the thermal ignition criticality are demonstrated.

1. Introduction

Analysis of possible development of runaway at production, storage, and use of a chemical product and subsequent choice of measures that can prevent an accident or mitigate its consequences are the important tasks of reaction hazards assessment [1]. The kinetic model of a reaction that describes heat generation plays a crucial role in the complete explosion model. Although thermal explosion has received much attention in the literature, the vast majority of investigations have been concerned with homogeneous boundary conditions ranging from the infinite Biot number case of a constant surface temperature [2] through a range of Biot numbers to zero [3]. In most of these studies, the determination of critical conditions that separate explosive and nonexplosive domains of a proceeding reaction and evaluation of induction period of an explosion if it appears has been the main focus. Moreover, two main approaches are used for obtaining the necessary data for critical condition. The first approach is based on direct determination of the explosion characteristics by means of explosive experiments. This approach is very expensive, dangerous, and time consuming [4]. The

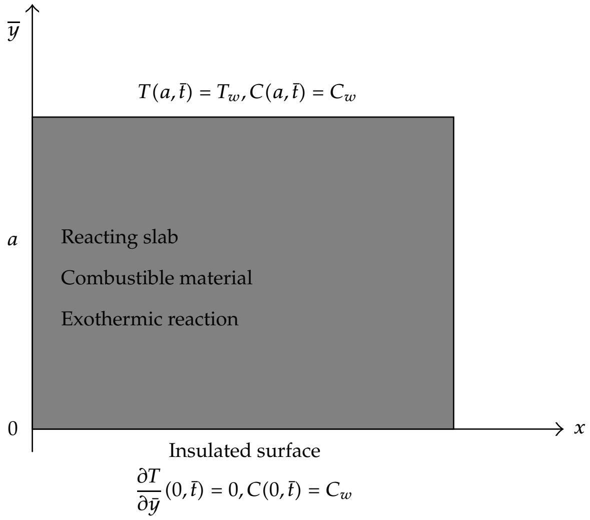


Figure 1: Geometry of the problem.

second approach involves the application of mathematical theory of thermal combustion. It involves derivation of appropriate mathematical models that allow major chemical and physical processes within an exothermic reacting system to be taken into account and application of sophisticated analytical and numerical techniques to tackle the problem. Several authors have analysed theoretically the problem of thermal explosion in a reacting slab; they include Zaturska and Banks [5], Bebernes and Eberly [6] and Makinde [7]. In all these earlier studies, the combined effect of asymmetric boundary condition and reactant consumption on the thermal ignition criticality has not been properly reported.

In the present study, the theoretical analysis of Makinde [7] is extended to include the effect of asymmetric boundary condition on both transient and steady-state exothermic *n*th-order oxidation reaction in a slab of combustible material with reactant consumption. This paper is organized as follows; firstly, the governing partial differential equations for oxidation reactions are presented and solved numerically using the semidiscretization finite difference technique known as method of lines. Secondly, the steady-state problem is tackled using perturbation technique coupled with a special type of the Hermite-Padé approximant in order to obtain the thermal criticality conditions in the system. Pertinent results are presented graphically and discussed quantitatively.

2. Mathematical Model

We consider the transient problem of combustible material undergoing an *n*th-order oxidation chemical reaction in a slab with insulated lower surface (see Figure 1). The complicated chemistry involved in this problem may be simplified by assuming a one-step finite-rate irreversible reaction given by

$$C_iH_j + \left(i + \frac{j}{4}\right)O_2 \longrightarrow iCO_2 + \frac{j}{2}H_2O + \text{Heat} \tag{2.1}$$

[Combustible material + Oxygen → Heat + Carbon dioxide + Water].

The dimensionless equations that describe the physical situation are given by [2, 3, 5–7]

$$\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial y^2} + \lambda(1+\varepsilon\theta)^m\phi^n e^{\theta/(1+\varepsilon\theta)}, \tag{2.2}$$

$$\alpha\frac{\partial\phi}{\partial t} = \frac{\partial^2\phi}{\partial y^2} - \lambda\beta(1+\varepsilon\theta)^m\phi^n e^{\theta/(1+\varepsilon\theta)}, \tag{2.3}$$

with initial and boundary conditions as

$$\theta(y,0) = 0, \qquad \phi(y,0) = 0, \tag{2.4}$$

$$\theta(1,t) = \theta_w, \qquad \phi(1,t) = 1, \tag{2.5}$$

$$\frac{\partial\theta}{\partial y}(0,t) = 0, \qquad \phi(0,t) = 1, \tag{2.6}$$

where λ is the Frank-Kamenetskii parameter, ε is the activation energy parameter, β is oxygen consumption rate parameter, α oxygen diffusivity parameter, n is the order of exothermic chemical reaction, and m is the numerical exponent given such that $m = \{-2, 0, 1/2\}$ represent numerical exponent for sensitised, Arrhenius, and bimolecular kinetics, respectively (see [6]). Equations (2.2)–(2.6) are obtained after introducing the dimensionless variables and quantities into the governing energy balance and concentration equations; that is,

$$\begin{gathered}\phi = \frac{(C-C_0)}{(C_w-C_0)}, \qquad \theta = \frac{E(T-T_0)}{RT_0^2}, \qquad \theta_w = \frac{E(T_w-T_0)}{RT_0^2}, \\ y = \frac{\overline{y}}{a}, \qquad t = \frac{k\bar{t}}{\rho c_p a^2}, \quad \varepsilon = \frac{RT_0}{E}, \\ \alpha = \frac{k}{D\rho c_p}, \qquad \beta = \frac{kRT_0^2}{DQE(C_w-C_0)}, \qquad \lambda = \frac{QAEa^2(C_w-C_0)^n}{kRT_0^2}\left[\frac{KT_0}{\upsilon l}\right]^m e^{-(E/(RT_0))},\end{gathered} \tag{2.7}$$

where T is the absolute temperature, $\bar{t}$ is the time, T_w is the slab upper surface temperature, C_w is the slab surface oxygen concentration, T_0 is the slab initial temperature, C_0 is the initial oxygen concentration in the material, θ is the dimensionless temperature, θ_w is the slab upper surface dimensionless temperature, ϕ is the dimensionless oxygen concentration, (x, y) represents the Cartesian coordinates, ρ is the density, c_p specific heat at constant pressure, k is the thermal conductivity of the material, Q is the exothermicity, A is the rate constant, E is the activation energy, R is the universal gas constant, l is the Planck number, K is the Boltzmann constant, υ is the vibration frequency, a is the slab width, $\overline{y}$ is the distance measured transverse direction, and D is the diffusivity of oxygen in the material.

3. Numerical Procedure

Here we employed the method of lines as our solution technique [8]. The governing equations (2.2)-(2.3) with the initial and boundary conditions (2.4)–(2.6) are transformed into a system of ODEs using finite differences for the spatial derivatives. Let $\Delta y = 1/N$, $y_i = (i-1)\Delta y$, $1 \le i \le N+1$; and $\theta_i(t)$, $\phi_i(t)$ represents $\theta(y_i, t)$, $\phi(y_i, t)$ respectively, then the semidiscrete system for the problem reads

$$\frac{d\theta_i}{dt} = \frac{1}{(\Delta y)^2}(\theta_{i+1} - 2\theta_i + \theta_{i-1}) + \lambda(1+\varepsilon\theta_i)^m \phi_i^n \left[e^{\theta_i/(1+\varepsilon\theta_i)}\right], \tag{3.1}$$

$$\alpha\frac{d\phi_i}{dt} = \frac{1}{(\Delta y)^2}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) - \lambda\beta(1+\varepsilon\theta_i)^m \phi_i^n \left[e^{\theta_i/(1+\varepsilon\theta_i)}\right], \tag{3.2}$$

with initial conditions

$$\theta_i(0) = 0, \qquad \phi_i(0) = 0, \quad 1 \le i \le N+1. \tag{3.3}$$

The first and last grid points are modified to incorporate the boundary conditions; that is,

$$\theta_1 = \theta_2, \qquad \theta_{N+1} = \theta_w, \tag{3.4}$$

$$\phi_1 = 1, \qquad \phi_{N+1} = 1. \tag{3.5}$$

The MAPLE program is employed to solve (3.1)–(3.5) using a fourth-order Runge-Kutta method.

4. Steady-State Analysis

A body of chemically reacting material releasing heat to its surroundings may achieve a safe steady state where the temperature of the body reaches some moderate value and stabilizes. Once a steady state is attained, (2.2)–(2.6) then become

$$\frac{d^2\theta}{dy^2} + \lambda(1+\varepsilon\theta)^m \phi^n e^{\theta/(1+\varepsilon\theta)} = 0, \tag{4.1}$$

$$\frac{d^2\phi}{dy^2} - \lambda\beta(1+\varepsilon\theta)^m \phi^n e^{\theta/(1+\varepsilon\theta)} = 0, \tag{4.2}$$

with

$$\theta(1) = \theta_w, \qquad \phi(1) = 1, \tag{4.3}$$

$$\frac{d\theta}{dy}(0) = 0, \qquad \phi(0) = 1. \tag{4.4}$$

The nonlinear nature of (4.1)–(4.4) precludes its exact solution. However, it is convenient to form a power series expansion in the Frank-Kamenetskii parameter; λ, that is,

$$\theta = \sum_{i=0}^{\infty} \theta_i \lambda^i, \qquad \phi = \sum_{i=0}^{\infty} \phi_i \lambda^i. \tag{4.5}$$

Substituting the solution series (4.5) into (4.1)–(4.4) and collecting the coefficients of like powers of λ, we obtained and solved the equations for the coefficients of solution series iteratively. The solutions for the temperature and the oxygen concentration in the slab are given as

$$\begin{aligned} \theta(y) &= \theta_w - \frac{\lambda}{2}(1+\varepsilon\theta_w)^m e^{\theta_w/(1+\varepsilon\theta_w)} \left(y^2-1\right) + O\left(\lambda^2\right), \\ \theta(y) &= 1 + \frac{\lambda\beta}{2}(1+\varepsilon\theta_w)^m e^{\theta_w/(1+\varepsilon\theta_w)} y(y-1) + O\left(\lambda^2\right). \end{aligned} \tag{4.6}$$

Using MAPLE, we obtained the first few terms of the above solution series. It is well known that this power series solution is valid for very small parameter values. However, by using the Hermite-Padé approximation technique [9], the usability of the solution series is extended beyond small parameter values as illustrated in the following section.

5. Thermal Criticality Determination

When the rate of heat generation in the reacting slab exceeds the rate of heat loss to the surroundings, then ignition can occur. Hence, the evaluation of critical regimes that separate the regions of explosive and nonexplosive ways of chemical reactions is extremely important from the application point of view. In order to achieve this goal, we employ a simple technique of series summation and improvement based on the generalization of Padé approximation technique (Baker and Graves-Morris [10]) and may be described as follows. Let

$$U_N(\lambda) = \sum_{i=0}^{N} a_i \lambda^i + O\left(\lambda^{N+1}\right), \quad \text{as } \lambda \longrightarrow 0, \tag{5.1}$$

be a given partial sum. It is important to note here that (5.1) can be used to approximate any output of the solution of the problem under investigation (e.g., the series for the wall heat flux parameter in terms of the Nusselt number $Nu = -d\theta/dy$ at y = 1), since everything can be Taylor expanded in the given small parameter. Assume the $U(\lambda)$ is a local representation of an algebraic function of λ in the context of nonlinear problems; we construct a multivariate series expression of the form

$$F_d(\lambda, U) = \sum_{m=1}^{d} \sum_{j=0}^{m} f_{m-j,j} \lambda^{m-j} U^j, \tag{5.2}$$

Table 1: Computations showing the criticality procedure rapid convergence ($\beta = n = 1, \theta_w = \varepsilon = 0$).

d	N	$Nu = -\theta'(1)$	λ_{cN}
2	4	2.293830707	1.07039427340
3	8	2.289550271	1.07040213355
4	13	2.289549038	1.07040198565
5	19	2.289549037	1.07040198791
6	26	2.289549037	1.07040198791

Table 2: Computations showing thermal ignition criticality for different parameter values.

β	n	θ_w	m	ε	$Nu = -\theta'(1)$	λ_c
0.1	1	0.0	0.0	0.00	2.025223122	0.8941780502
0.5	1	0.0	0.0	0.00	2.134510046	0.9640287456
1.0	1	0.0	0.0	0.00	2.289549037	1.0704019879
0.1	3	0.0	0.0	0.00	2.074810972	0.9265325131
0.1	5	0.0	0.0	0.00	2.122974429	0.9600824416
0.1	1	0.5	0.0	0.00	2.025223122	0.5423464026
0.1	1	1.0	0.0	0.00	2.025223122	0.3289497214
0.1	1	0.0	0.5	0.01	2.057311239	0.8993850447
0.1	1	0.0	−2.0	0.01	2.112233348	0.9231510103
0.1	1	0.0	0.0	0.01	2.068063491	0.9040392715
0.1	1	0.0	0.0	0.10	2.600639145	1.0110740529

of degree $d \geq 2$, such that

$$\frac{\partial F_d}{\partial U}(0,0) = 1, \qquad F_d(\lambda, U_N) = \mathrm{O}\left(\lambda^{N+1}\right), \quad \text{as } \lambda \longrightarrow 0. \tag{5.3}$$

The requirement (5.3) yields $f_{0,1} = 1$ ensuring that the polynomial F_d has only one root which vanishes at $\lambda = 0$ and reduces the problem to a system of N linear equations for the unknown coefficients of F_d. The entries of the underlying matrix depend only on the N given coefficients a_i in (5.1); consequently, we take $N = (d^2 + 3d - 2)/2$, so that the number of equations equals the number of unknowns. The polynomial F_d is a special type of the Hermite-Padé approximant [7, 9, 11] and is then investigated for bifurcation and criticality conditions using the Newton diagram [12]. The chief merit of this method is its ability to reveal the solution branches, criticality values as well as extending the usability of the power series solution beyond small parameter values.

6. Results and Discussion

Computational results in Table 1 illustrate the rapid convergence of Hermite-Padé approximation procedure highlighted in the above section with gradual increase in the number of series coefficients utilized for the approximants. In Table 2, we observed that the magnitude of thermal ignition criticality (λ_c) increases with an increase in the parameter values of, β, n, ε and a decrease in the slab upper surface temperature parameter θ_w. Consequently, a delay in the development of thermal runaway in the reacting slab will be experienced, hence, enhances thermal stability of the system. Moreover, it is noteworthy from Table 2 that

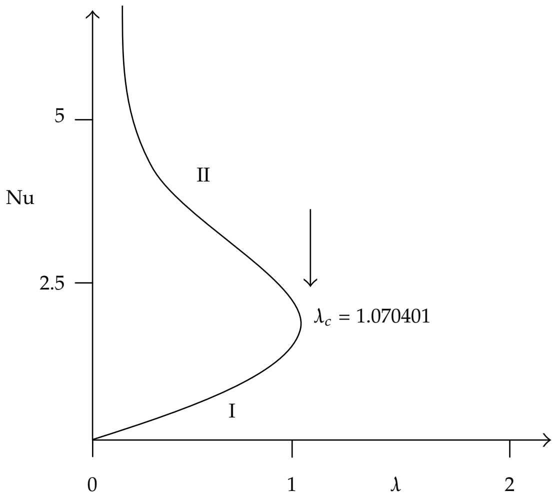
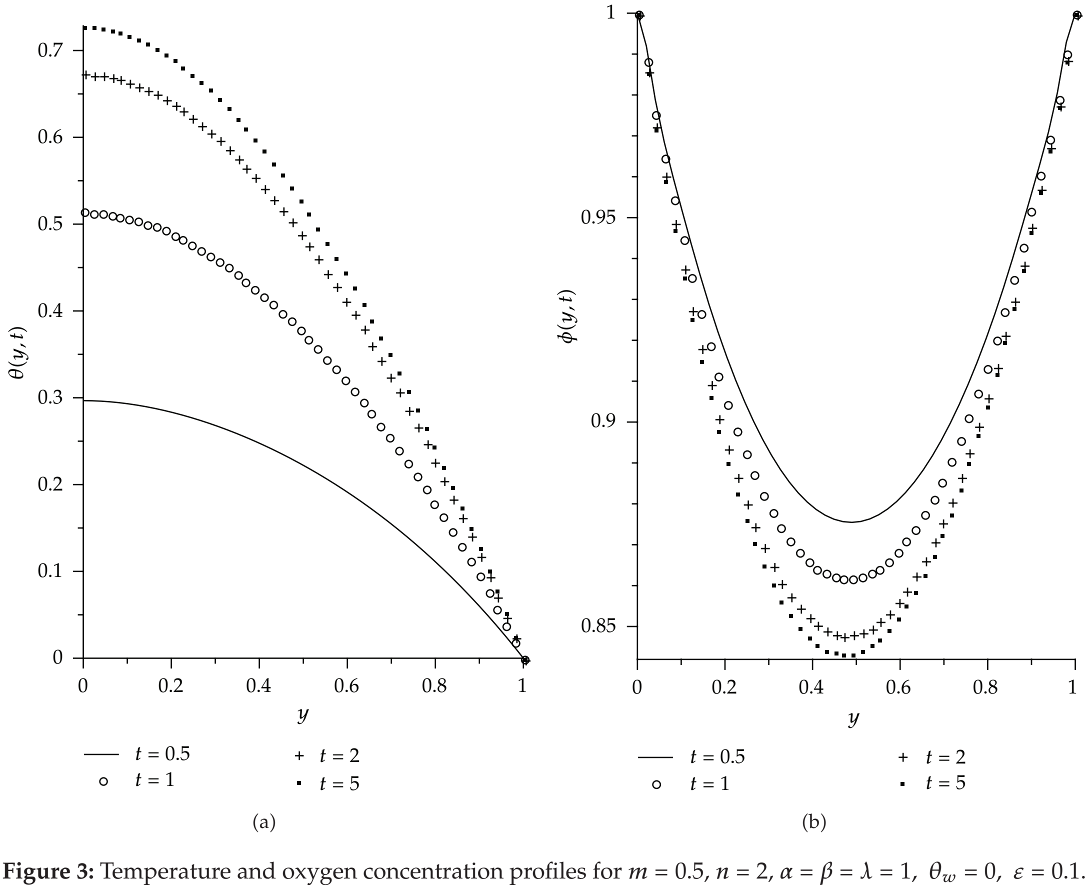


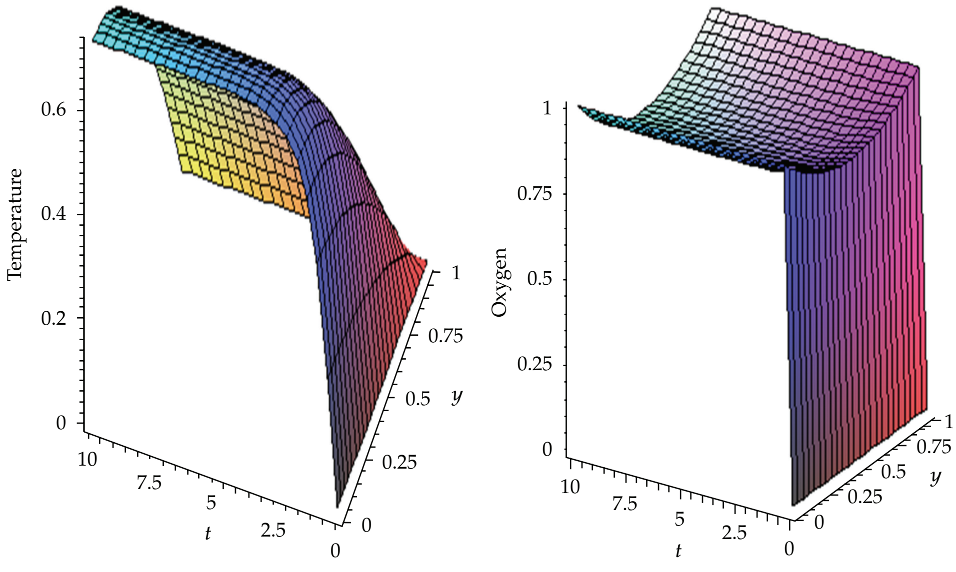
Figure 2: A slice of approximate bifurcation diagram in the $(\lambda, Nu(\beta = n = 1, \theta_w = \varepsilon = 0))$ plane.



(a)

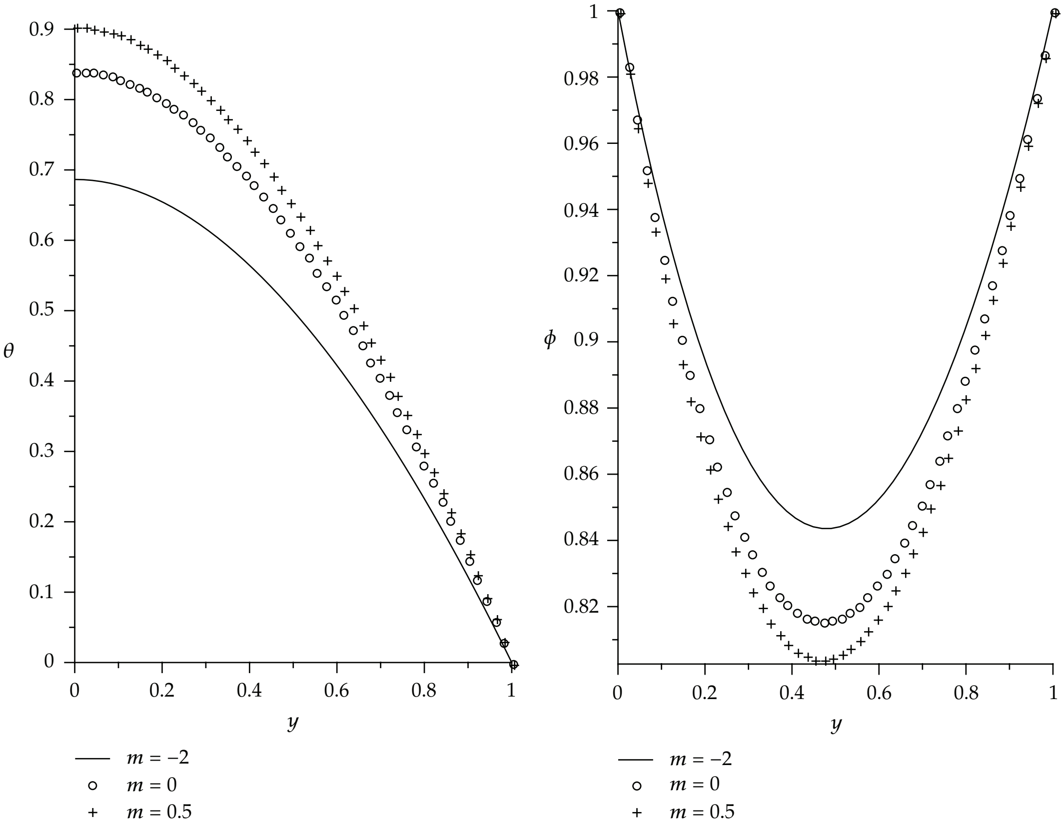
(b)

Figure 3: Temperature and oxygen concentration profiles for $m = 0.5$, $n = 2$, $\alpha = \beta = \lambda = 1$, $\theta_w = 0$, $\varepsilon = 0.1$.



(a) (b)

Figure 4: Temperature and oxygen concentration profiles for $m = 0.5$, $n = 2$, $\alpha = \beta = \lambda = 1$, $\theta_w = 0$, $\varepsilon = 0.1$.



(a) (b)

Figure 5: Temperature and oxygen concentration profiles for $n = \beta = \lambda = 1$, $\theta_w = 0$, $\varepsilon = 0.1$.

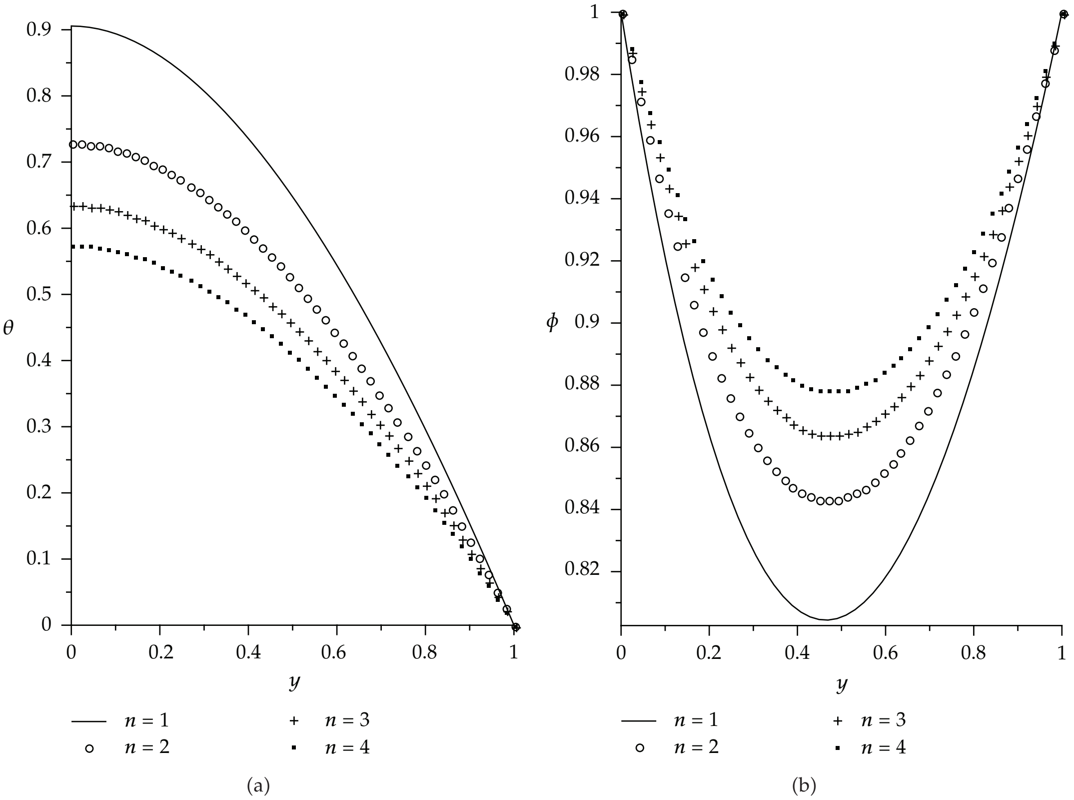


Figure 6: Temperature and oxygen concentration profiles for $m = 0.5,\ \lambda = \beta = 1,\ \theta_w = 0,\ \varepsilon = 0.1$.

thermal ignition occur faster in a bimolecular ($m = 0.5$) type of exothermic oxidation reaction as compared to the Arrhenius ($m = 0$) and sensitised ($m = -2$) type of reaction.

A slice of the bifurcation diagram for $0 \leq \varepsilon \ll 1$ in the (λ, Nu) plane is shown in Figure 2. It represents the qualitative change in the thermal system as parameter λ increases. In particular, for $0 \leq \varepsilon \ll 1$, $\beta > 0$, and $n > 0$, there is a critical value λ_c (a turning point) such that, for $0 < \lambda < \lambda_c$, there are two solutions (labeled I and II). The upper and lower solution branches occur due to nonlinearity in model equations for energy and concentration balance. When $\lambda > \lambda_c$ the system has no real solution and displays a classical form indicating thermal runaway. As exothermic reaction due to oxidation chemical kinetics increases, the slab temperature increases uncontrollably until it ignites.

6.1. Effect of Various Parameters on Temperature and Oxygen Concentration Profiles

The effects of various thermophysical parameters on the slab temperature and oxygen concentration profiles are displayed in Figures 3, 4, 5, 6, 7, 8, and 9. Generally, the temperature is maximum at the slab lower insulated surface and decreases transversely with minimum value at its upper surface. Meanwhile, the oxygen concentration is lowest along the slab centerline ($y = 0.5$) and maximum at the slab surfaces. This can be attributed to the fact that oxygen is utilized within the slab during exothermic chemical kinetics and fresh

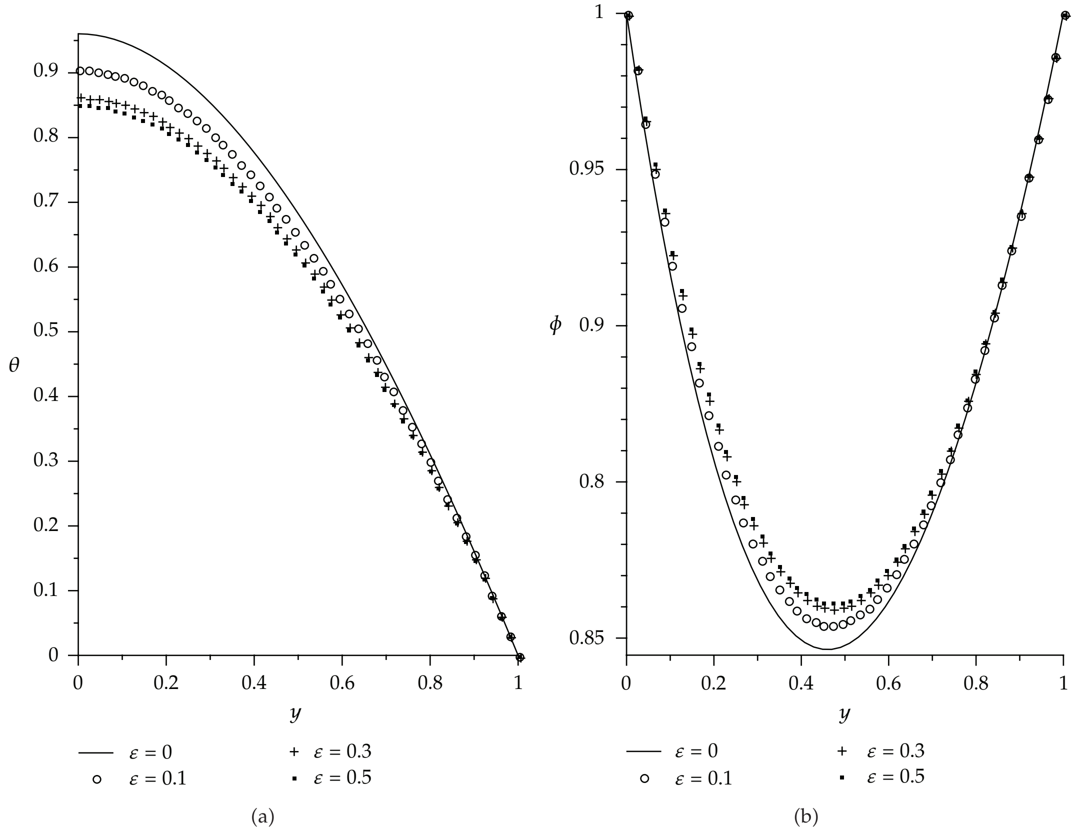
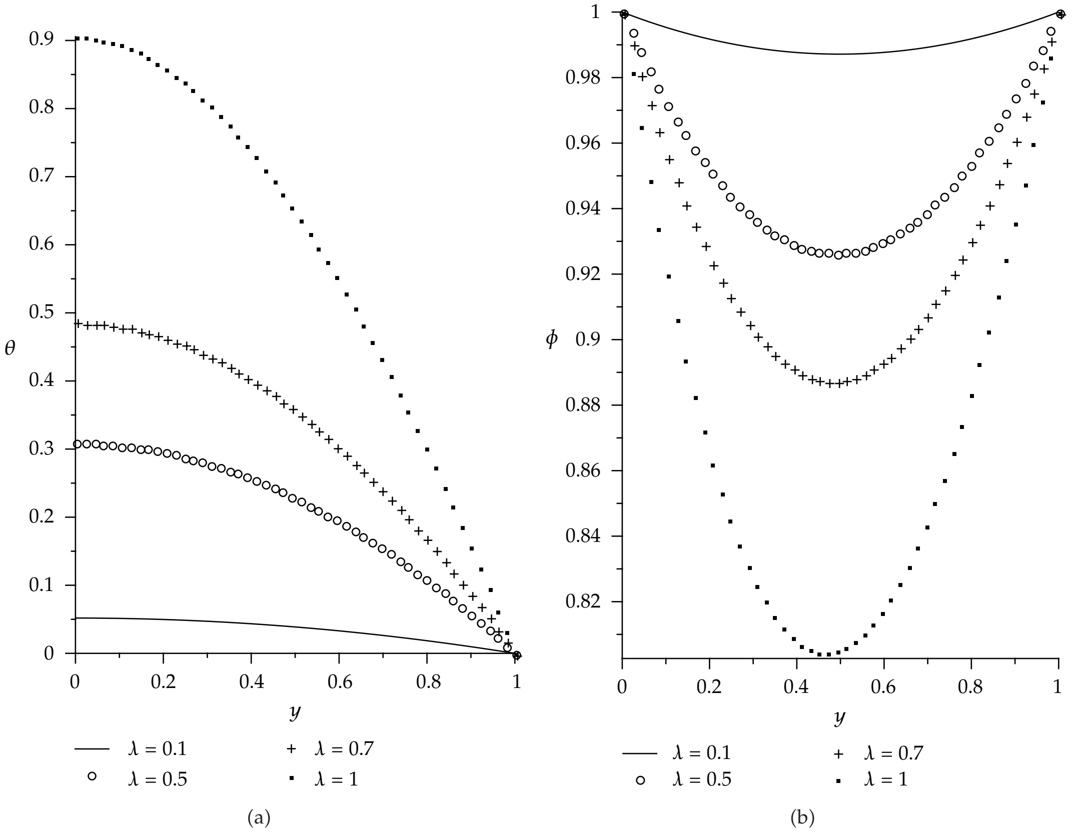


Figure 7: Temperature and oxygen concentration profiles for $m = 0.5$, $n = \lambda = \beta = 1$, $\theta_w = 0$.

supply of oxygen from the surrounding is obtained at the slab surfaces. The evolution of the temperature and oxygen concentration in the slab is illustrated in Figures 3 and 4. It is noteworthy that the slab temperature increases while the oxygen concentration decreases gradually with time until it attains its steady-state value. Once the steady-state value is attained, the slab temperature and oxygen concentration remain the same for a given set of parameter values with respect to a further increase in time. In Figure 5, we observed that the slab temperature is highest during bimolecular reaction ($m = 0.5$) and lowest for sensitized reaction ($m = -2$), hence confirming the earlier results in Table 2. Consequently, oxygen concentration in the slab is lowest during bimolecular reaction and highest for sensitized reaction. In Figures 6 and 7, we observed that the slab temperature decreases while oxygen concentration increases with an increase in the reaction order index (n) and activation energy parameter (ε). This clearly implies that a higher-order exothermic oxidation chemical reaction will be more thermally stable than a lower one. Figures 8 and 9 illustrated the effect of the Frank-Kamenetskii parameter (λ) and the slab upper surface temperature parameter (θ_w) on the slab temperature and oxygen concentration. The slab temperature increases while the oxygen concentration decreases with an increase in the parameter values of λ and θ_w. As λ and θ_w increase, the oxygen consumption within the slab increases and the slab internal heat generation due to exothermic oxidation reaction increases, this invariably leads to an elevation in the slab temperature.



(a)

(b)

Figure 8: Temperature and oxygen concentration profiles for $m = 0.5$, $n = \beta = 1$, $\theta_w = 0$, $\varepsilon = 0.1$.

7. Conclusions

We have computationally investigated the one-step nth -order oxidation exothermic reaction in a slab with an insulated lower surface and an isothermal upper surface. The model, which consists of a system of coupled heat and mass transfer differential equations, has been solved numerically using a semi-discretization technique and analytical using a perturbation technique coupled with a special type of the Hermite-Padé approximants. Our results revealed, among others, the thermal ignition criticality conditions and with the right combination of thermophysical parameters controlling the system, the thermal runaway can be prevented.

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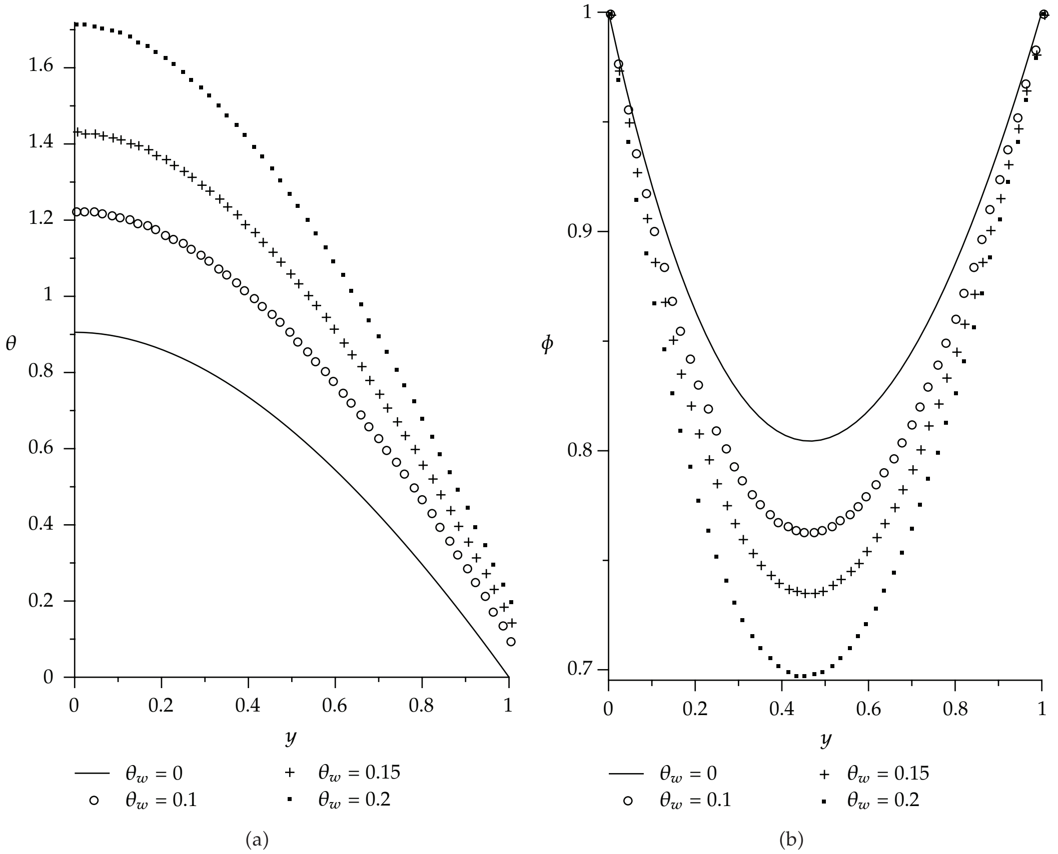

(a)

(b)

Figure 9: Temperature and oxygen concentration profiles for $m = 0.5$, $n = \lambda = \beta = 1$, $\varepsilon = 0.1$.

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