

Thermal explosion analysis of a strong exothermic chemical reaction with variable pre-exponential factor in a spherical vessel

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ABSTRACT

This study is devoted to investigate the analysis of thermal explosion of a strong exothermic chemical reaction with variable pre-exponential factor in a spherical vessel. The steady state solutions for strong exothermic decomposition of a combustible material uniformly distributed in a heated spherical vessel under Bimolecular, Arrhenius and Sensitised reaction rates. Analytical solutions are constructed for the governing nonlinear boundary-value problem using perturbation technique together with a special type of Hermite-Padé approximants and important properties of the temperature field including bifurcations and thermal criticality are discussed.

Keywords: Thermal explosion, Exothermic reaction, Spherical vessel, Variable pre-exponential factor, Hermite-Padé approximants

INTRODUCTION

The thermal explosion theory is the spontaneous explosion due to internal heating in combustible materials such as industrial waste fuel, coal, hay, wool wastes and so on. Infact, the problem of evaluation of critical regimes thought of as regimes separating the regions of explosive and non explosive ways of chemical reactions are the main mathematical problem of the thermal explosion theory (see [1-3]). The analyses of these problems have been performed based on close-form, approximation and phase-plane methods and numerical techniques using computational fluid dynamics packages. Okoya [4] investigated reactive-diffusive equation with variable pre-exponential factor, taking the diffusion of the reactant in a slab into account. He presented a new analytical solution for the Frank Kamenetskii parameter δ in the special case corresponding to the Sensitised reaction. Makinde [5], examined steady state solutions for the strongly exothermic decomposition of a combustible material uniformly distributed in a heated cylindrical pipe under Bimolecular, Arrhenius and Sensitised reaction rates, neglecting the consumption of the material. Recently, Adegbe and Alao [6], studied thermal explosion of sensitised reaction with variable heat loss in a slab. To the best of authors' knowledge, the temperature field effect of the thermal stability of combustible material in a spherical vessel has not been investigated theoretically. This particular problem is extremely useful in handling and transporting explosive materials in engineering and petrochemical industries.

This present work extends the theoretical study of Makinde [5] to thermal explosion of a strong exothermic chemical reaction in a spherical vessel which makes Makinde [5] a special type of ours. In the following section, the problem is formulated, analysed and discussed.

Mathematical Analysis: It is assumed that the combustible material inside the cylindrical vessel is subject to a steady state one step exothermic chemical reaction with possibility of variable heat loss to the surrounding. The equation of the heat balance in the original variables in which heat exchange between the reacting material and the spherical vessel walls together with the boundary conditions can be written as [3]

$$\frac{k}{r^2} \frac{d}{dr} \left(r^{-2} \frac{dT}{dr} \right) + QC_0 A \left(\frac{KT}{vh} \right)^m \exp\left(-\frac{E}{RT}\right) = 0, \quad (2.1)$$

$$\frac{dT}{dr}(0) = 0, \quad T(a) = T_0, \quad (2.2)$$

where T is the absolute temperature, T_0 the wall temperature, k the thermal conductivity of the material, Q the heat of reaction, A the rate constant, E the activation energy, R the universal gas constant, C_0 the initial concentration of the reactant species, h the Planck's number, K the Boltzmann's constant, ν vibration frequency, a the pipe radius, r the radial distance measured normal direction, z the pipe axial distance, α the convection coefficient, A and V the surface area and volume of the cylindrical pipe and m is the numerical exponent such that $m = \{-2, 0, \frac{1}{2}\}$ represent numerical exponent for Sensitised,

Arrhenius and Bimolecular kinetics respectively (see [7]). We introduce the following dimensionless variables into Eqs. (2.1)- (2.2)

$$\theta = \frac{E(T-T_0)}{RT_0^2}, \quad \varepsilon = \frac{RT_0}{E}, \quad r = \frac{\bar{r}}{a}, \quad \lambda = \frac{QEAd^2 K^m T_0^{m-2} e^{-\frac{E}{RT_0}}}{v^m h^m Rk}, \quad (2.3)$$

and obtaining the dimensionless governing equation together with the corresponding boundary conditions as

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\theta}{dr} \right) + \lambda (1 + \varepsilon\theta)^m \left(e^{\frac{\theta}{1+\varepsilon\theta}} \right) = 0, \quad (2.4)$$

$$\frac{d\theta}{dr}(0) = 0, \quad \theta(1) = 0, \quad (2.5)$$

where λ , ε , δ represents the Frank Kamenetskii, activation energy and heat loss parameters respectively. In the following section, Eqs. (2.4) and (2.5) are solved using both perturbation and multivariate series summation techniques (see [8-10]).

Method of Solution: To solve Eqs. (2.4) and (2.5), it is convenience to take a power series expansion in the Frank Kamenetskii parameter λ , i.e.

$$\theta = \sum_{i=0}^{\infty} \theta_i \lambda^i. \quad (3.1)$$

Substitute the solution series into Eqs. (2.4)- (2.5) and collecting the coefficients of like power of λ , we obtained and solved the equations governing the coefficients of solution series. The solution for the temperature field for Sensitised, Arrhenius and Bimolecular reaction rates are given as

$$\theta(r; \lambda, \varepsilon, m = -2) = -\frac{\lambda}{8}(r^2 - 1) + \frac{\lambda^2}{144}(r^2 - 1)(r^2 - 1)(2\varepsilon - 1) + \frac{\lambda^3}{2304}(r^2 - 1)(-21r^4\varepsilon + 4r^4 + 21r^4\varepsilon^2 + 84r^2\varepsilon - 17r^2 - 84r^2\varepsilon^2 + 31\varepsilon^2 - 31\varepsilon + 13) + 0(\lambda^4) \quad (3.2)$$

$$\theta(r; \lambda, \varepsilon, m = 0) = -\frac{\lambda}{8}(r^2 - 1) + \frac{\lambda^2}{144}(r^2 - 1)(r^2 - 1)(2\varepsilon - 1) + \frac{\lambda^3}{2304}(r^2 - 1)(-4r^4 + 3r^4\varepsilon - 16r^2\varepsilon + 17r^2 + 11\varepsilon - 13) + 0(\lambda^4) \quad (3.3)$$

$$\theta(r; \lambda, \varepsilon, m = 1/2) = -\frac{\lambda}{8}(r^2 - 1) + \frac{\lambda^2}{288}(r^2 - 1)^2(2\varepsilon - 1) + \frac{\lambda^3}{5184}(r^2 - 1)(3r^4\varepsilon - 16r^4 + r^4\varepsilon^2 + 4r^2\varepsilon + 90r^2 + r^2\varepsilon^2 - 12\varepsilon^2 - 48\varepsilon - 52) + 0(\lambda^4) \quad (3.4)$$

We use computer symbolic algebra package (MAPLE), we obtained the first twenty terms of the above solution series as well as the series for maximum cylindrical pipe temperature $\theta_{max} = \theta(0)$. We know that power series solution is valid for very small parameter values, however, using Hermite-Padé approximation technique [12, 13], we have

extended the usability of the solution series beyond small parameter values as illustrated in the following section.

Thermal Stability Analysis: It is important to know that the evaluation of critical regimes thought of as a regime separating the regions of explosive and non-explosive ways of chemical reactions is extremely important from the application point of view. This characterizes the thermal stability properties of the reacting materials under consideration and the onset of thermal explosion in the system. In order to achieve this goal, we employ a special type of Hermite-Padé approximation technique [5, 12, 13]. Suppose that the partial sum

$$U_{N-1}(\lambda) = \sum_{i=0}^{N-1} a_i \lambda^i = U(\lambda) + O(\lambda^N) \text{ as } \lambda \rightarrow 0, \quad (4.1)$$

is given. It is important to note here that Eq. (4.1) can be used to evaluate any output of the solution of the problem under investigation (e.g. the series for the maximum temperature $\theta_{max} = \theta(0)$), since everything can be Taylor expanded in the given small parameter. Assume $U(\lambda)$ is a local representation of an algebraic function of λ in the context of nonlinear problems, we construct an expression of the form

$$F_d(\lambda, U) = \sum_{i=1}^d \sum_{k=0}^i f_{i-k,k} \lambda^{i-k} U^k, \quad (4.2)$$

of degree $d \geq 2$, such that

$$\frac{\partial F_d}{\partial U}(0,0) = 1 \text{ and } F_d(\lambda, U_N) = O(\lambda^{N+1}), \text{ as } \lambda \rightarrow 0. \quad (4.3)$$

The requirement (4.3) 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_n and we shall 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 Hermite-Padé approximant and is then investigated for bifurcation and criticality conditions using Newton diagram [14].

RESULTS AND DISCUSSION

The procedure in section 4 above is applied on the first 19 terms of the solution series and we obtained the results as shown in tables (1) and (2) below:

Table 1: Computations showing the procedure rapid convergence for $\varepsilon = 0.0$, $m = -2, 0, 1/2$

D	N	θ_{max}	λ_c	α_{cN}
1	9	1.58684089840758	3.09999999999999	0.499999999999999
2	12	1.58649458367141	3.10000000000000	0.500000000000000
3	15	1.58649459231122	3.10000000000000	0.500000000000000
4	18	1.58649459231122	3.10000000000000	0.500000000000000
5	21	1.58649459231122	3.10000000000000	0.500000000000000

Table 2: Computation showing criticality for Sensitized, Arrhenius and Bimolecular reaction

M	ε	θ_{max}	λ_c	α_{cN}
-2, 0, 1/2	0.0	1.58649459231122	3.10000000000000	0.500000000000000
-2	0.1	3.74319645303452	4.201346310876	0.500000000000000
0.0	0.1	2.98420314510674	3.361275381367	0.500000000000000
0.5	0.1	2.64453843125073	3.213460813467	0.500000000000000

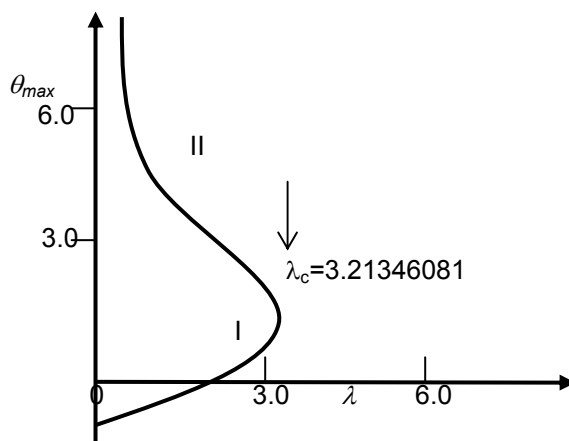


Fig. 1. A slice of approximate bifurcation diagram in the $(\lambda, \theta_{max} (, m = 0.5, \varepsilon = 0.1))$ plane

Table (1) shows the rapid convergence of the dominant singularity λ_c i.e. the value of thermal criticality in the system together with its corresponding maximum temperature θ_{max} as the number of series coefficients utilized in the approximants increases. Table 2, illustrates the variation in the values of thermal criticality conditions (λ_c) for different combination of embedded parameters. At very large activation energy ($\varepsilon=0$), thermal explosion criticality is independent of the type of reaction as shown in Eq. (2.4). It is interesting to note from the table (2) that explosion in bimolecular reaction will occur faster than in Arrhenius and Sensitized reactions. This can be attributed to the lower thermal criticality value of bimolecular reaction.

The magnitude of thermal criticality increases with a increase in the activation energies, thus preventing the early development of thermal runaway and enhancing thermal stability A slice of the bifurcation diagram for (λ, θ_{max}) plane is shown in Fig. (1). It represents the variation of spherical vessel maximum temperature (θ_{max}) with the Frank-Kamenetskii parameter (λ). In particular, for every $0 \leq \varepsilon \leq 0.1$ there is a critical value λ_c (a turning point) such that, for $0 \leq \lambda < \lambda_c$ there are two solutions (labelled I and II). The upper and lower solution branches occur due to chemical kinetics in the governing heat balance equation (Eq. 2.4). When λ_c

$< \lambda$ the system has no real solution and displays a classical form indicating thermal runaway.

CONCLUSION

In this paper an analysis has been carried out to study the thermal development in a spherical vessel with one step exothermic chemical reaction, taking into account the temperature dependent variable pre-exponential factor. The nonlinear governing equation is solved using perturbation technique coupled with a special type of Hermite- Padé approximants. We obtain accurately the thermal criticality conditions as well as the solution branches. Our results reveal among others that the thermal runaway in the system is delayed due to the vessel used compared with the results in the literatures. Hence, with the proper choice of thermophysical parameters, the thermal stability can be enhanced.

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