EXOTHERMIC EXPLOSIONS IN A SLAB: A CASE STUDY OF SERIES SUMMATION TECHNIQUE

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ABSTRACT

This paper examine the steady-state solutions for the strongly exothermic decomposition of a combustible material uniformly distributed between symmetrically heated parallel plates under Bimolecular, Arrhenius and Sensitised reaction rates, neglecting the consumption of the material. 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: Multivariate algebraic approximation, Thermal explosions, Bifurcation.

1. INTRODUCTION: The problem of evaluation of critical regimes thought of as regimes separating the regions of explosive and non-explosive ways of chemical reactions is the main mathematical problem of the thermal explosion theory ([1], [2]). The classical formulation of this problem is first introduced by Frank-Kamenetskii ([2]). Neglecting the reactant consumption, the equation for the heat balance in the original variables together with the boundary conditions can be written as

$$k\frac{d^2T}{d\bar{y}^2} + QC_0 A\left(\frac{KT}{\upsilon h}\right)^m e^{-\frac{E}{RT}} = 0, \ \frac{dT}{d\bar{y}}(0) = 0, \ T(a) = T_0 \tag{1}$$

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, υ vibration frequency, a the slab half width, $\bar{y}$ is distance measured in the normal direction to the plane and m is the numerical exponent such that $m=\{-2, 0, \frac{1}{2}\}$ represent numerical exponent for Sensitised, Arrhenius and Bimolecular kinetics respectively ([1],[2]). Following [2], we introduce the following dimensionless variables in equation (1):

$$\theta = \frac{E(T-T_0)}{RT_0^2}, \ \varepsilon = \frac{RT_0}{E}, \ y = \frac{\bar{y}}{a}, \ \lambda = \frac{QEAa^2C_0K^mT_0^{m-2}e^{-\frac{E}{RT_0}}}{\upsilon^m h^m Rk}, \tag{2}$$

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

$$\frac{d^2\theta}{dy^2} + \lambda(1+\varepsilon\theta)^m e^{\left(\frac{\theta}{1+\varepsilon\theta}\right)} = 0, \ \frac{d\theta}{dy}(0) = 0, \ \theta(1) = 0, \tag{3}$$

where λ, ε represent the Frank-Kamenetskii and activation energy parameters respectively. In the following sections, equation (3) is solved using both perturbation and multivariate series summation techniques ([3],[4],[5]).

2. PERTURBATION TECHNIQUE: To solve equations (3), it is convenient to take a power series expansion in the Frank-Kamenetskii parameter λ, i.e., $\theta = \sum_{i=0}^{\infty}\theta_i\lambda^i$. Substitute the solution series into equation (3) and collecting the coefficients of like powers of λ, we obtained and solved the equations governing the coefficients of solution series. The solution for the temperature field for Sensitized, Arrhenius and Bimolecular reaction rates are given as

$$\theta(y;\lambda,\varepsilon,m=-2) = -\frac{\lambda}{2}(y^2-1) - \frac{\lambda^2}{24}(y^2-1)(y^2-5)(2\varepsilon-1) + \frac{\lambda^3}{360}(y^2-1)(-11y^4\varepsilon \tag{4a}$$

$$+2y^4 + 11y^4\varepsilon^2 + 64y^2\varepsilon - 13y^2 - 64y^2\varepsilon^2 + 221\varepsilon^2 - 221\varepsilon + 47) + O(\lambda^4)$$

$$\theta(y;\lambda,\varepsilon,m=0) = -\frac{\lambda}{2}(y^2-1) + \frac{\lambda^2}{24}(y^2-1)(y^2-5) + \frac{\lambda^3}{360}(y^2-1)(-2y^4 \tag{4b}$$

$$+3y^4\varepsilon - 12y^2\varepsilon + 13y^2 + 33\varepsilon - 47) + O(\lambda^4)$$

$$\theta(y;\lambda,\varepsilon,m=1/2) = -\frac{\lambda}{2}(y^2-1) - \frac{\lambda^2}{48}(y^2-1)(y^2-5)(2+\varepsilon) + \frac{\lambda^3}{1440}(y^2-1)(4y^4\varepsilon \tag{4c}$$

$$-8y^4 + y^4\varepsilon^2 + 4y^2\varepsilon + 52y^2 + y^2\varepsilon^2 - 14\varepsilon^2 - 56\varepsilon - 188) + O(\lambda^4)$$

Using computer symbolic algebra package (MAPLE), we obtained the first 21 terms of the above solution series (4) as well as the series for maximum fluid temperature $\theta_{max} = \theta(y=0;\lambda,\varepsilon,m)$.

3. BIFURCATION STUDY: The main tool of this paper is a simple technique of series summation based on a special type of Hermite-Padé approximation technique and may be described as follows. Let us suppose that the partial sum

$$U_{N-1}(\lambda) = \sum_{i=0}^{N-1} a_i \lambda^i = U(\lambda) + O(\lambda^N) \quad \text{as } \lambda \to 0, \tag{5}$$

is given, we construct a multivariate series expression of the form

$$F_d(\lambda, U_{N-1}) = A_{0N}(\lambda) + A_{1N}^d(\lambda)U^{(1)} + A_{2N}^d(\lambda)U^{(2)} + A_{3N}^d(\lambda)U^{(3)}, \tag{6}$$

whereby, we substitute in equation (6) $U^{(1)} = U$, $U^{(2)} = U^2$, $U^{(3)} = U^3$ for cubic algebraic approximant and $U^{(1)} = U$, $U^{(2)} = DU$, $U^{(3)} = D^2U$, $D=d/d\lambda$ for second order differential approximant, such that

$$A_{0N}(\lambda) = 1, \quad A_{iN}(\lambda) = \sum_{j=1}^{d+i} b_{ij}\lambda^{j-1}, \text{ and } F_d(\lambda, U) = O(\lambda^{N+1}) \text{ as } \lambda \to 0, \tag{7}$$

and $d \geq 1$, $i =1, 2, 3$. The condition (7) nomalises the F_d, reduces the problem to a system of N linear equations for the unknown coefficients of F_d and ensures that the order of series A_{iN} increases as i and d increase in value. We shall take $N=3(2+d)$, so that the number of equations equals the number of unknowns. The algebraic approximant enables us to obtain the solution branches while the dominant singularity or criticality in the problem is obtained easily using the differential approximant. For details on the above procedure, interested readers can see ([3], [4], [5]). Using the above procedure on the solution series in section (2), we obtained the results as shown in table (1) below:

Table (1): Computation showing criticality for Sensitised, Arrhenius and Bimolecular reaction (N=21)

m	ε	θ_{max}	λ_c
-2.0, 0.0, 0.5	0.0	1.186842168	0.8784576797
-2.0	0.1	2.222393808	1.3138875302
0.0	0.1	1.524355912	0.9882078037
0.5	0.1	1.420243862	0.9322160716

4. RESULTS AND CONCLUSIONS: From table (1) above, we observe that at very large activation energy, thermal explosions criticality is independent of the type of reaction. However, for moderately large value of activation energy, the criticality varies from one reaction to another. Explosion in Bimolecular reaction seems to occur faster than in Arrhenius and Sensitised reactions. Two solution branches (type I and II) are identified with a bifurcation point at λ_c as shown in a sketch of bifurcation diagram in figure (1) below. Finally, the above series summation procedure can be used as an effective tool to investigation several other parameter dependent nonlinear boundary-value problems.
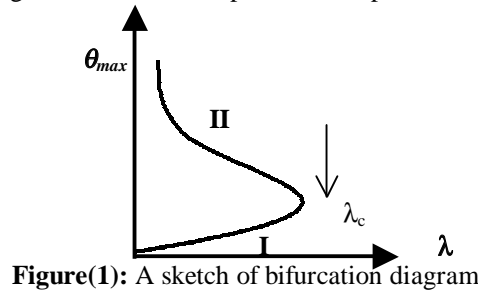
Figure(1): A sketch of bifurcation diagram

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