EXOTHERMIC EXPLOSIONS IN SYMMETRIC GEOMETRIES:
AN EXPLOITATION OF PERTURBATION TECHNIQUE

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In this paper, the steady-state solutions for the strongly exothermic decomposition of a combustible material uniformly distributed in heated symmetrical geometries under Arrhenius kinetics, neglecting the consumption of the material, are examined. Analytical solutions are constructed for the governing nonlinear boundary-value problem using perturbation technique together with a special type of Hermite-Pade approximants and important properties of the temperature field including bifurcations and thermal criticality are discussed.

Key words: Exothermic reaction, Arrhenius kinetics, Symmetric geometries, Hermite-Pade approximants.


1. INTRODUCTION

The phenomena of spontaneous explosion due to internal heating in combustible materials such as industrial waste fuel, coal, hay, wool waste, etc. can be described by thermal explosion theory. In fact, 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 [1–4]. The classical formulation of this problem is first introduced by Frank-Kamenetskii [3]. Neglecting the reactant consumption, the equation for the heat balance in the original variables together with the boundary conditions can be written as

\[
\frac{1}{r^m} \frac{d}{dr} \left( r^n \frac{dT}{dr} \right) + \frac{QC_0A}{k} e^{-\frac{E}{RT}} = 0, \quad \frac{dT}{dr}(0) = 0, \quad T(a) = T,
\]

where \( T \) is the absolute temperature, \( T_0 \) the geometry 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, $a$ the geometry half width, $r$ the radial distance measured in the normal direction and $m$ is the symmetry geometries exponent such that $m = \{0, 1, 2\}$ represent Slab, Cylindrical and Spherical geometries respectively [1–4]. Following [3], we introduce the following dimensionless variables in equation (1):

$$\theta = \frac{E(T - T_0)}{RT_0^2}, \quad \delta = \frac{RT_0}{E}, \quad r = \frac{r}{a}, \quad \lambda = \frac{QEAa^2C_0e^{-\frac{E}{RT_0}}}{T_0^2 RK},$$

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

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

where $\lambda$, $\delta$ represent the Frank-Kamenetskii and activation energy parameters respectively. In the following sections equation (3) is solve for large activation energy i.e. $\delta = 0$ using both perturbation and multivariate series summation techniques [5–7].

2. METHOD OF SOLUTION

To solve equation (3), it is convenient to take a power series expansion in the Frank-Kamenestskii parameter $\lambda$, 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 $\lambda$, we obtained and solved the equations governing the coefficients of solution series. The solution for the temperature field for Slab, Cylindrical and Spherical geometries are given as

$$\theta(r; \lambda, m = 0) = -\frac{\lambda}{2}(r^2 - 1) + \frac{\lambda^2}{24}(r^2 - 1)(y^2 - 5) + \frac{\lambda^3}{360}(r^2 - 1)(-2r^4 + 13r^2 - 47) + O(\lambda^4) \quad (4)$$

$$\theta(r; \lambda, m = 1) = -\frac{\lambda}{4}(r^2 - 1) + \frac{\lambda^2}{64}(r^3 - 1)(r^2 - 3) + \frac{\lambda^3}{2304}(r^2 - 1)(-3r^4 + 15r^2 - 30) + O(\lambda^4) \quad (5)$$

$$\theta(r; \lambda, m = 2) = -\frac{\lambda}{6}(r^2 - 1) + \frac{\lambda^2}{360}(r^2 - 1)(3r^2 - 7) - \frac{\lambda^3}{7560}(r^2 - 1)(4r^4 - 17r^2 + 25) + O(\lambda^4). \quad (6)$$
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 $\theta_{\text{max}} = \theta(r = 0; \lambda)$.

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

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

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

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

whereby, we substitute in equation (9) $U^{(1)} = U$, $U^{(2)} = U^2$, $U^{(3)} = U^3$ 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

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

and $d \geq 1$, $i = 1, 2, 3$. The condition (9) normalizes 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 [5–7].

5. RESULTS AND DISCUSSION

The bifurcation procedure above is applied on the first 44 terms of the solution series and we obtained the results as shown in Tables 1 and 2 below.

Table 1 shows the rapid convergence of the dominant singularity $\lambda_c$, i.e., the thermal criticality in the flow field together with its corresponding critical exponent $\alpha_c$ and maximum temperature $\theta_{\text{max}}$ with gradual increase in the number of series coefficients utilized in the approximants for Table 2 above, we observe
that at very large activation energy, thermal explosions criticality varies from one symmetric geometry to another. Our results agree perfectly well with all the earlier results obtained for similar geometries, (see [1–4]). However, our bifurcation procedure produces more accurate results as compare to what has already been reported in the literature. For a Slab and cylindrical geometries, two solution branches (type I and II) are identified with a bifurcation point at $\lambda_c$ (see Fig. 1a), however, for a spherical geometry further multiplicity of solution branches is observed as shown in the bifurcation diagram in Fig. 1b with additional transitional turning point at $\lambda_{tc} = 1.664$ below.

\textbf{Table 1}

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\textbf{d} & \textbf{N} & \textbf{$\theta_{max}$} & \textbf{$\lambda_c$} & \textbf{$\alpha_c/N$} \\
\hline
1 & 9 & 1.186841989 & 0.878451473 & 0.4999999 \\
2 & 12 & 1.186842168 & 0.8784576797 & 0.5000000 \\
3 & 15 & 1.186842168 & 0.8784576797 & 0.5000000 \\
\hline
\end{tabular}
\caption{Computations Showing the Procedure Rapid Convergence for $\varepsilon = 0.0, m = 0$}
\end{table}

\textbf{Table 2}

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{Geometries} & \textbf{m} & \textbf{$\theta_{max}$} & \textbf{$\alpha_c$} \\
\hline
Slab & 0 & 1.1868421686343890972358527550 & 0.8784576797812903015519592733 \\
Cylinder & 1 & 1.3862943611198906188344642429 & 2.0000000000000000000000000000 \\
Sphere & 2 & 1.6074567750838420289452538542 & 3.3219921183398239884164780820 \\
\hline
\end{tabular}
\caption{Computations showing the maximum temperature and thermal criticality for ($N = 44$)}
\end{table}

\textbf{Fig. 1.} – A sketch of bifurcation diagram, (a) Slab & Cylinder, (b) Sphere.

\section{5. CONCLUSIONS}

A bifurcation study by analytic continuation of a power series in the bifurcation parameter for a particular solution branch is utilized to investigate the
probable of strong exothermic explosions in symmetrical geometries. For large activation energy, the procedure reveals accurately the steady state thermal criticality conditions as well as the solution branches. Finally, the above series summation procedure can be used as an effective tool to investigate several other parameter dependent nonlinear boundary value problems.

REFERENCES