EFFECT OF GOEMETRY ON THE ANALYSIS OF THERMAL EXPLOSION OF A STRONGLY EXOTHERMIC CHEMICAL REACTONS

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ABSTRACT

This study is devoted to investigate the effect of geometry on thermal explosion of a strong exothermic chemical reaction with variable pre-exponential factor under Bimolecular, Arrhenius and Sensitised reaction rate, 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 Hermite-pade approximation and important properties of the temperature field including bifurcations and thermal criticality are discussed. It is shown that temperature field is highly influenced by the geometry.

Key words: Geometry; thermal expansion; exothermic chemical reaction; variable pre-exponential factor.

1. INTRODUCTION

The thermal expansion theory is the spontaneous explosion due to internal heating in combustible materials such as industrial waste fuel, coal, hay, wool wastes and so on. 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 are the main mathematical problem of the thermal explosion theory (see [1-10]).

The analyses of these problems have been performed based on closed-form, approximation and phase-plane methods and numerical techniques using computational fluid dynamics packages. [10], examined reactive-diffusive equation with variable pre-exponential factor, taking the diffusion of the reactant in a slab into account. He presented boundary conditions of a generalised lane-emden equation of the second-kind. To the best of author's knowledge, the thermal explosion analysis has not been considered for a spherical shape under Bimolecular, Arrhenius and sensitised reaction rate.

In this work, we extend [8-10] to thermal explosion of a strong exothermic chemical reaction in a slab, a cylindrical pipe and a spherical pipe. In the following section, the problem is formulated, analysed and discussed.

2. MATHEMATICAL ANALYSIS

The geometry of the problem is depicted in Figure 1. It is assumed that the combustible material inside the slab, cylindrical and spherical pipes are subjected to a steady state one step exothermic chemical reaction with possibility of variable pre-exponential factors.

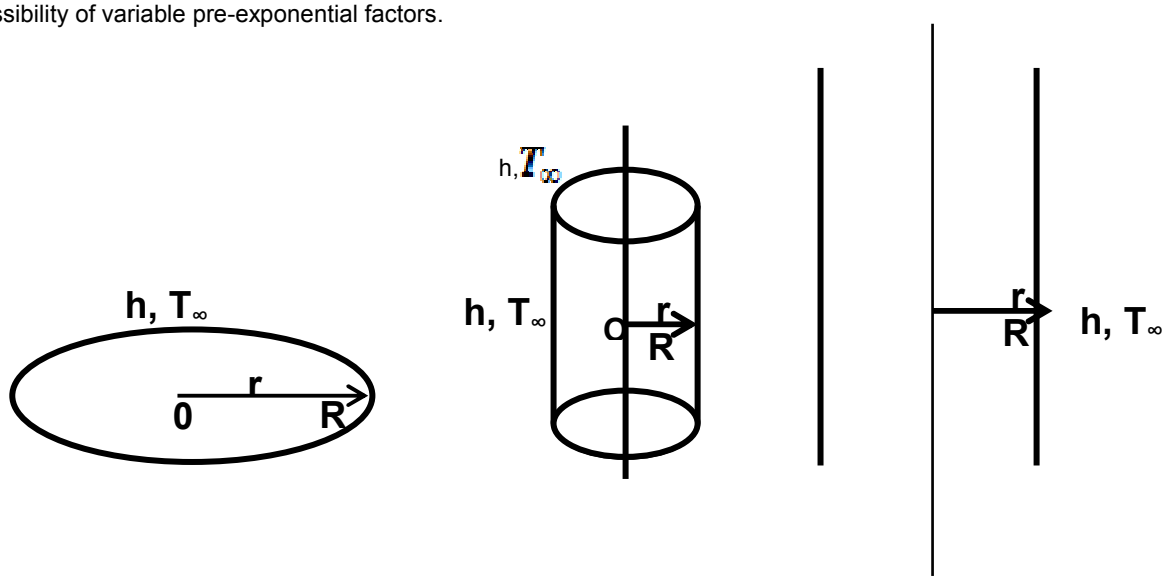

Fig 1. *Geometry of the problem*

The equation of the heat balance in the original variables together with the boundary conditions can be written as (see[4])

$$\frac{K}{\bar{r}^n}\frac{d}{d\bar{r}}(\bar{r}^n\frac{dT}{d\bar{r}})+QC_0A(\frac{KT}{vh})^m\exp[-E/RT]=0 \tag{2.1}$$

$$\frac{dT}{d\bar{r}}(0)=0,\qquad T(0)=T_0 \tag{2.2}$$

Where T is the absolute temperature, T_0 the wall temperature, k the thermal conductivity of the materials, 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, v the vibration frequency, a the pipe radius, $\bar{r}$ the radial distance measured normal direction, n the geometry of the vessel i.e. n=0 (slab), n=1 (cylinder) and n=2 (spherical0 and m the numerical exponent such that $m=\{-2,0,1/2\}$ represent numerical exponent for sensitised, Arrhenius and Bimolecular kinetics respectively (see[8] and [2]). We introduce the following dimensionless variables into equation (2.1)-(2.2)

$$\theta=\frac{E(T-T_0)}{RT_0^2},\qquad \varepsilon=\frac{RT_0}{E},\qquad r=\frac{\bar{r}}{a},\quad \lambda=\frac{QEAa^2K^mT_0^{m-2}e^{-E/RT_0}}{v^mh^mRK}$$
$$\sigma=\frac{v^m\,\mathrm{Re}^{E/RT_0}}{QEAK^mT_0^{m-2}}, \tag{2.3}$$

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

$$\frac{1}{r^n}\frac{d}{dr}(r^n\frac{d\theta}{dr})+\lambda(1+\varepsilon\theta)^me^{\theta/1+\varepsilon\theta}=0 \tag{2.4}$$

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

Where λ,ε represent the Frank Kamenetskii and activation energy parameters respectively. In the following sections, equations (2.4)-(2.5) are solved using both perturbation and multivariate series summation techniques (see [8-9])

3. METHOD OF SOLUTION

To solve equations (2.4)-(2.5), it is convenient to take a power series expansion in the Frank Kamanetskii parameter λ i.e.

$\theta=\sum_{i=0}^{\infty}\theta_i\lambda_i$. Substitute the solution series into equations (2.4)-(2.5) and collecting the coefficients of like powers of λ , we obtained and solved the equations governing the coefficients of solution series. The solutions for the temperature field for sensitized, Arrhenius and Bimolecular reaction rates are given as

$$\theta(r;\lambda,\varepsilon,m=-2,n=0)=-\frac{\lambda}{2}(y^2-1)-\frac{\lambda^2}{24}(y^2-1)(y^2-5)(2\varepsilon-1)$$
$$+\frac{\lambda^3}{360}(y^2-1)(-11y^4\varepsilon+2y^4+11y^4\varepsilon^2+64y^2\varepsilon-13y^2-64y^2\varepsilon^2 \tag{3.1a}$$
$$+221\varepsilon^2-221\varepsilon+47)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=0,n=0)=-\frac{\lambda}{2}(y^2-1)+\frac{\lambda^2}{24}(y^2-1)(y^2-5)$$
$$+\frac{\lambda^3}{360}(y^2-1)(-2y^4+3y^4\varepsilon-12y^2\varepsilon+13y^2+33\varepsilon \quad (3.1b)$$
$$-47)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=1/2,n=0)=-\frac{\lambda}{2}(y^2-1)-\frac{\lambda^2}{48}(y^2-1)(y^2-5)(2+\varepsilon)$$
$$+\frac{\lambda^3}{1440}(y^2-1)(4y^4\varepsilon-8y^4+y^4\varepsilon^2+4y^2\varepsilon+52y^2+y^2\varepsilon^2 \quad (3.1c)$$
$$-14\varepsilon^2-56\varepsilon-188)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=-2,n=1)=-\frac{\lambda}{4}(r^2-1)-\frac{\lambda^2}{64}(r^2-1)(r^2-3)(2\varepsilon-1)$$
$$-\frac{\lambda^3}{2304}(r^2-1)(-16r^4\varepsilon+3r^4+16r^4\varepsilon^2+74r^2\varepsilon-15r^2-74r^2\varepsilon^2 \quad (3.1d)$$
$$+142\varepsilon^2-142\varepsilon+30)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=0,n=1)=-\frac{\lambda}{4}(r^2-1)+\frac{\lambda^2}{64}(r^2-1)(r^2-3)$$
$$+\frac{\lambda^3}{2304}(r^2-1)(-3r^4+4r^4\varepsilon-14r^2\varepsilon+15r^2 \quad (3.1e)$$
$$+22\varepsilon-30)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=1/2,n=1)=-\frac{\lambda}{4}(r^2-1)+\frac{\lambda^2}{128}(r^2-1)(r^2-3)(2+\varepsilon)$$
$$+\frac{\lambda^3}{9216}(r^2-1)(4r^4\varepsilon-12r^4+r^4\varepsilon^2+4r^2\varepsilon+60r^2+r^2\varepsilon^2 \quad (3.1f)$$
$$-88\varepsilon^2-32\varepsilon-120)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=-2,n=2)=-\frac{\lambda}{8}(r^2-1)+\frac{\lambda^2}{144}(r^2-1)(r^2-1)(2\varepsilon-1)$$
$$+\frac{\lambda^3}{2304}(r^2-1)(-21r^4\varepsilon+4r^4+21r^4\varepsilon^2+84r^2\varepsilon-17r^2-84r^2\varepsilon^2 \quad (3.1l)$$
$$+31\varepsilon^2-31\varepsilon+13)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=0,n=2)=-\frac{\lambda}{8}(r^2-1)+\frac{\lambda^2}{144}(r^2-1)(r^2-1)(2\varepsilon-1)$$
$$+\frac{\lambda^3}{2304}(r^2-1)(-4r^4+3r^4\varepsilon-16r^2\varepsilon+17r^2 \quad (3.1J)$$
$$+11\varepsilon-13)+0(\lambda^4)$$

$$\theta(r;\lambda,\varepsilon,m=1/2,n=2)=-\frac{\lambda}{8}(r^2-1)+\frac{\lambda^2}{288}(r^2-1)^2(2\varepsilon-1)$$
$$+\frac{\lambda^3}{5184}(r^2-1)(3r^4\varepsilon-16r^4+r^4\varepsilon^2+4r^2\varepsilon+90r^2+r^2\varepsilon^2 \quad (3.1K)$$
$$-12\varepsilon^2-48\varepsilon-52)+0(\lambda^4)$$

Using computer symbolic algebra package (MAPLE), we obtained the first 30 terms of the above solution series (3.1a)-(3.3k) as well as the series for maximum fluid temperature $\theta_{\max}=\theta(r=0;\lambda,\varepsilon,m)$

4. BIFURCATION STUDY

The main tool of this paper is a simple technique of series summation based on the generalized of Pade approximants and may be described as follows.

Let us suppose that the partial sum

$$U_{N-1}(\lambda)=\sum_{i=0}^{N-1}a_i\lambda_i=U(\lambda)+0(\lambda^N)\ \ as\ \ \lambda\to 0 \quad (4.1)$$

is given. We are concerned with the bifurcation study by analytic continuation as well as the dominant behaviour of the solution by using partial sum (4.1). We expect that the accuracy of the critical parameters will ensure the accuracy of the solution. It is well known that the dominant behaviour of a solution of a differential equation can often be written as

$$U(\lambda)\approx\begin{cases}K(\lambda_c-\lambda)^{\alpha} & for\ \ \alpha\neq 0,1,2,3.....\\ & as\lambda\to\lambda_c\\ K(\lambda_c-\lambda)^{\alpha}\left|k\right\|\lambda_c-\lambda| & for\alpha=0,1,2,3.....\end{cases} \quad (4.2)$$

Where K is some constant and λ_c is the critical point with the exponent α. However, we shall make the simplest hypothesis in the contest of nonlinear problems by assuming the $U(\lambda)$ is the local representation of an algebraic function of λ.

Therefore, we seek an expression of the form

$$F_d(\lambda,U_{N-1})=A_{0N}(\lambda)+A_{1N}^d(\lambda)U^{(1)}+A_{2N}^d(\lambda)U^{(2)}+A_{3N}^d(\lambda)U^{(3)} \quad (4.3)$$

Such that

$$A_{0N}(\lambda)=1,\qquad A_{1N}(\lambda)=\sum_{j=1}^{d+i}b_{ij}\lambda^{j-1} \quad (4.4)$$

And

$$F_d(\lambda,U)=0(\lambda^{N+1})\quad as\qquad \lambda\to 0 \quad (4.5)$$

Where $d\geq 1,\ i=1,2,3.$ the condition (4.4) normalizes the F_d and ensures that the order of series A_{iN} increases as $i\ and\ d$ increase in value. There are thus $3(2+d)$ undetermined coefficients b_{ij} in the expression (4.4). The requirement (4.5) 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. Henceforth, we shall take

$$N=3(2+d) \quad (4.6)$$

So that the number of equations equal the number of unknowns. Equation (4.5) is a new special type of Hermite-Pade approximants. Both the algebraic and differential approximants form of equation (4.5) are considered. For instance, we let

$$U^{(1)}=U,\qquad U^{(2)}=U^2\ ,\ U^{(3)}=U^3 \quad (4.7)$$

And obtain a cubic Pade approximant. This enables us to obtain solution branches of the underlying problem in addition to the one represented by the original series. In the same manner, we let

$$U^{(1)}=U,\quad U^{(2)}=DU,\quad U^{(3)}=D^2U \quad (4.8)$$

In equation (4.4), where D is the differential operator given by $D = \frac{d}{d\lambda}$. This leads to a second order differential approximants. It is an extension of the integral approximants idea by [12] and enables us to obtain the dominant singularity in the flow fluid i.e. by equating the coefficient $A_{3N}(\lambda)$ in the equation (4.5) to zero. Meanwhile, it is very important to know that the rationale for chosen the degrees of A_{iN} in equation (4.4) in this particular application is based on the simple technique of singularity determination in second order linear ordinary differential equation with polynomial coefficients as well as the possibility of multiple solution branches for the nonlinear problem (see [13]).

In practice, one usually finds that the dominant singularities are located at zeroes of the second order linear ordinary differential equation. Hence, some of the zeroes of $A_{3N}^{d}(\lambda)$ may provide approximations of the singularities of the series U and we expect that the accuracy of the singularities will ensure the accuracy of the approximants.

The critical exponent α_N can easily be found by using Newton's polygon algorithm. However, it is well known that, in the case of algebraic equations, the only singularities are structurally stable have simple turning points. Hence, in practice, one almost invariably obtains $\alpha_N = 1/2$. If we assume a singularity of algebraic type as in equation (4.2), then the exponent may be approximated by

$$\alpha_N = 1 - \frac{A_{2N}(\lambda_{CN})}{DA_{3N}(\lambda_{CN})} \tag{4.9}$$

For details on the above procedure, interested readers can see (see [8-11]). We apply this procedure on the first 30 terms of the solution series as shown in following section.

5. RESULTS AND DISCUSSION

The bifurcation procedure above is applied on the first 30 terms of the solution series and we obtained the results as shown in Tables 1-6.

Tables 1-3 shows the rapid convergence of the dominant singularity λ_c i.e the thermal criticality in the flow field together with its corresponding critical exponent α_c and maximum temperature $\theta_{\max}$ with gradual increase in the number of series coefficients utilized in the approximants. Two solution branches (type I and II) are identified with a bifurcation point at λ_c (i.e. turning point) as shown in a sketch of bifurcation diagram in Figure 2. Note that, at very large activation energy, thermal explosion criticality is independent of the type of reaction as shown in Table 1-3. For moderately value of activation energy, the criticality varies from one reaction to another as shown in Tables 4-6. Explosion in Bimolecular reaction seems to occur faster than in Arrhenius and Sensitised reactions. Note that the interesting part of this analysis from table 6 shows that the temperature is maximum and the thermal criticality is also maximum which means that despite the fact that the temperature is high, the explosion rate is very slow compare to table 4 and table 5. It is clearly seen that the thermal runaway is controlled by the geometrical shape of the explosive mechanism.

Table 1. Computations showing the procedure rapid convergence for ε = 0, m = -2, 0, ½, n = 0

D	N	$\theta_{\max}$	λ_c	α_{cN}
1	9	1.186841989	0.8784514732	0.4999999
2	12	1.186842168	0.8784576797	0.5000000
3	15	1.186842168	0.8784576797	0.5000000
4	18	1.186842168	0.8784576797	0.5000000
5	21	1.186842168	0.8784576797	0.5000000

Table 2. Computations showing the procedure rapid convergence for ε = 0, m = -2, 0, ½, n = 1

D	N	$\theta_{\max}$	λ_c	α_{cN}
1	9	1.386540594	1.999999999	0.499999999
2	12	1.386294350	2.000000000	0.500000000
3	15	1.386294361	2.000000000	0.500000000
4	18	1.386294361	2.000000000	0.500000000
5	21	1.386294361	2.000000000	0.500000000

Table 3. Computations showing the procedure rapid convergence for ε = 0, m = -2, 0, ½, n = 2

D	N	$\theta_{\max}$	λ_c	α_{cN}
1	9	1.586840898	3.099999999	0.499999999
2	12	1.586494584	3.100000000	0.500000000
3	15	1.586494592	3.100000000	0.500000000
4	18	1.586494592	3.100000000	0.500000000
5	21	1.586494592	3.100000000	0.500000000

Table 4. Computations showing Criticality for Sensitised, Arrhenius and Bimolecular Reaction, n =0

M	ε	$\theta_{\max}$	λ_c	α_{cN}
-2, 0.0, 0.5	0.0	1.186842168	0.8784576797	0.500000000
-2	0.1	2.222393808	1.3138875302	0.500000000
0.0	0.1	1.524355912	0.9882078037	0.500000000
0.5	0.1	1.420243862	0.9322160716	0.500000000

Table 5. Computations showing Criticality for Sensitised, Arrhenius and Bimolecular Reaction, n =1

M	ε	$\theta_{\max}$	λ_c	α_{cN}
-2, 0.0, 0.5	0.0	1.386294361	2.0000000000	0.500000000
-2	0.1	2.654197458	3.0162070811	0.500000000
0.0	0.1	1.802469335	2.2612754821	0.500000000
0.5	0.1	1.677326619	2.1321950843	0.500000000

Table 6. Computations showing Criticality for Sensitised, Arrhenius and Bimolecular Reaction, n =2

M	ε	$\theta_{\max}$	λ_c	α_{cN}
-2, 0.0, 0.5	0.0	1.586494592	3.1000000000	0.500000000
-2	0.1	3.743196453	4.2013463134	0.500000000
0.0	0.1	2.984203145	3.3612753815	0.500000000
0.5	0.1	2.644538431	3.2034608115	0.500000000

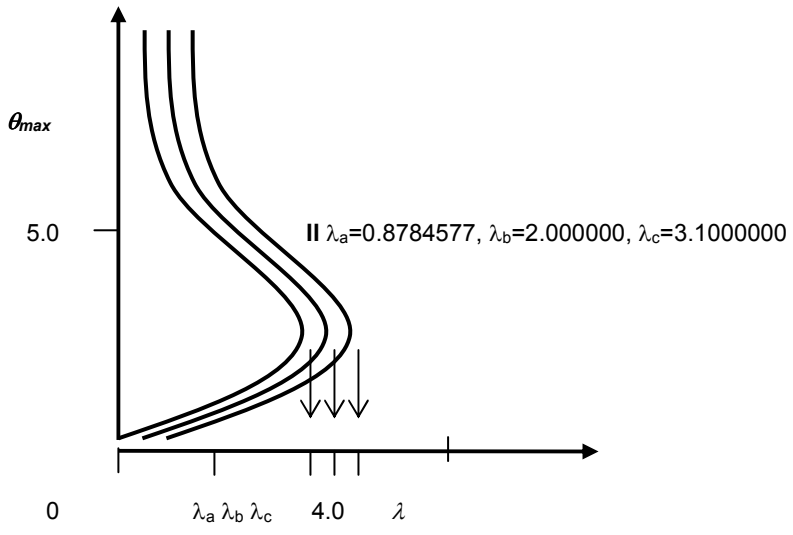

Fig. 2. *A slice of approximate bifurcation diagram in the (λ , θ_{max} (δ = 0.1, m = 0.5, ε = 0.1)) plane*

6. 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 effect of geometry on the analysis of thermal explosion of strong

exothermic chemical reactions. For large activation energy, the procedure reveals accurately the steady state thermal criticality conditions as well as the solution branches.

It was shown that geometry has a greater influence on the thermal runaway of an explosive mechanism.

Finally, the above series summation procedure can be used as an effective tool to investigate several other parameter dependent nonlinear boundary-value problems

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