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Hermite-Padé approximation approach to exothermic explosions with heat loss

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Abstract. We consider in this study the steady-state solutions for the exothermic chemical reaction in a slab, taking into account the heat loss to the ambient and assuming an Arrhenius-type temperature dependence. Analytical solutions are obtained for the governing nonlinear boundary value problem using the homotopy analysis method. A special type of Hermite-Padé approximation is used to extract numerical estimations of the critical Frank-Kamenetskii parameters and the critical temperatures. The consequences of heat loss are explored within the framework of a one dimensional, steady state model.

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1. Introduction

Study of thermal explosion of combustible materials intended at ensuring the safety of their storage, transportation and use is an important practical aspect of evaluating and controlling the hazard. The basic theory of the phenomenon of thermal explosion was initiated by Semenov [1] and Frank-Kamenetskii [2] has developed the quasi-stationary theory of thermal explosion in order to determine the critical conditions that separate explosive and non-explosive domains of an ongoing reaction. Many researchers ([3]-[12] and related references therein) have then generalized the theory of Frank- Kamenestkii with various stages of heat transfer around the reactive material. These include cases where the surface temperature is connected to the surrounding environment by a convective heat transfer.

We assume that the material is motionless and that the heat losses are determined by the thermal conductivity of the material [8]. In this study, the steady-state solutions are investigated in a slab obeying an Arrhenius law, with a temperature dependence of the pre-exponential factor $A(T)$ and ignoring the consumption of the material.

Analytical solutions are constructed using homotopy analysis method [13]. The critical values of the temperature field and of the Frank- Kamenestkii parameter are obtained using a special type of Hermite-Padé approximants [10].

The structure of this paper is as follows. Section 2 presents the boundary value problem governing the ignition of a combustible material in a slab. In section 3, we will apply the homotopy analysis method to this nonlinear boundary value problem. Section 4 is assigned to a brief description of the Hermite-Padé approximation and its application to calculate bifurcation points. The last section is devoted to the results

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obtained by the proposed method and to a comparison with other works. Conclusions will appear in Section 6.

2. Mathematical formulation

According to the relation given by Frank-Kamenetskii for a one-dimensional steady combustion and assuming that the chemical reaction can be represented by an Arrhenius rate law, the equation of heat balance in the original variables can be written as:

$$k\frac{d^2T}{dx^2} + \rho QA\left(\frac{KT}{\nu h\rho}\right)^m exp\left(-\frac{E}{RT}\right) - \alpha\frac{S}{V}(T - T_0) = 0 \tag{1}$$

together with the following boundary conditions, meaning that the walls are maintained at a fixed temperature T_0 throughout the process:

$$T = T_0 \text{ on } x = a. \tag{2}$$

In these equations, k is the thermal conductivity of the material, Q is the heat of reaction, A is the reaction rate constant, ν is the vibration frequency, h is the Plank's constant, ρ is the density, $m \in \{-2, 0, 0.5\}$ is a numerical exponent corresponding respectively to the sensitized, Arrhenius and bimolecular temperature dependence (cf. Boddington et al. [4]), K is the Boltzmann's constant, E is the activation energy, R is the universal gas constant, α is the convection coefficient, a is the geometry half width, S/V is the surface area to volume ratio of the slab and T_0 is the absolute temperature of the surrounding environment.

We introduce the following dimensionless variables:

$$\overline{x} = \frac{x}{a},\ \theta = \frac{R(T - T_0)}{RT_0^2},\ \epsilon = \frac{RT_0}{E},\ \delta = \frac{a^2\rho QEAK^mT_0^{m-2}e^{\frac{-E}{RT_0}}}{(\rho h\nu)^m Rk},\ \beta = \frac{\alpha S}{akT_0}$$

to obtain

$$\frac{d^2\theta}{d\overline{x}^2} + \delta\,(1 + \epsilon\theta)^m exp\left(\frac{\theta}{1 + \epsilon\theta}\right) - \beta\theta = 0 \tag{3}$$

$$\theta = 0 \text{ on } \overline{x} = 1 \tag{4}$$

where δ, ϵ, β represent respectively the Frank-Kamenetskii, the dimensionless activation energy and the heat loss parameters. Hereafter, we will drop the bar symbol for clarity.

3. Method of solution

In this section, we apply the homotopy method [13] for solving the problem (3)-(4). Let us define the following linear operator:

$$L = \frac{d^2}{dx^2} - \beta id \tag{5}$$

If $\hbar$ denotes a non-zero auxiliary parameter and $u_0(x)$ an initial guess of θ, we can construct the zero-order deformation equation as:

$$(1-p)\left(L(u(x,p)) - L(u_0(x))\right) = p\hbar\left[L(u(x,p)) + \delta\,(1 + \epsilon u(x,p))^m exp\left(\frac{u(x,p)}{1 + \epsilon u(x,p)}\right)\right] \tag{6}$$

with the following boundary conditions:

$$u(x,p) = 0 \text{ on } \quad x = \pm 1 \tag{7}$$

where p is an embedding parameter. When $p = 0$, a straightforward calculation gives

$$u(x, 0) = u_0(x).$$

When $p = 1$, the zero-order deformation equations (6) and (7) are equivalent to the original Eqs. (3) and (4) and we obtain:

$$u(x, 1) = \theta(x). \tag{8}$$

Thus, changing p from 0 to 1 is equivalent to transforming $u(x, p)$ from $u_0(x)$ to $\theta(x)$. We can expand $u(x, p)$:

$$u(x, p) = u_0(x) + \sum_{n=1}^{\infty} p^n u_n(x) \tag{9}$$

Assuming that the above series is convergent when $p = 1$ and using Eq. (8), we obtain:

$$\theta(x) = u_0(x) + \sum_{n=1}^{\infty} u_n(x) \tag{10}$$

We will take an initial approximation $u_0(x) = 0$ which is in fact the solution of the linear problem. We substitute relation (9) into the governing equation (6)-(7), and collecting the coefficients of like powers of p to obtain a sequence of differential equations and boundary conditions. We now successively have:

$$u_1(x) = \frac{1}{2}\hbar(x^2 - 1)$$

$$u_2(x) = \frac{1}{24}\hbar(x^2 - 1)\left[\delta\hbar(x^2 - 5)(\epsilon m + 1) + \beta(5 - x^2) + 12)(\hbar + 1)\right]$$

and so on. As pointed by Liao [13], the auxiliary parameter $\hbar$ can be employed to adjust the convergence region of the series (9). For this purpose, the $\hbar$-curves of $\theta''(1)$ are displayed in Figure 1 for 10th and 15th approximation order. It is clear from this figure that the range for the admissible values for $\hbar$ is $-1.42 \le \hbar \le -0.61$.

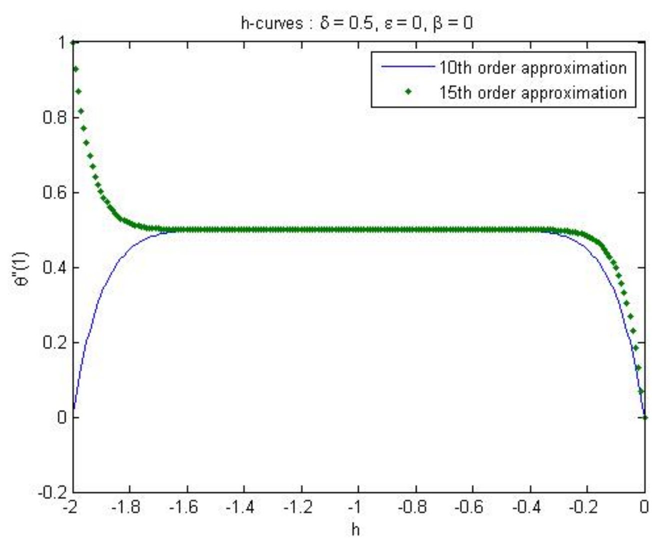

FIGURE 1. $\hbar$-curves for $\theta''(1)$, solid line: 10th-order approximation; dashed line: 15th-order approximation.

4. Hermite - Padé approximation technique

There is a critical value for the Frank- Kamenetskii parameter δ_c, meaning that no steady state is possible and that a reaction runaway can occur. One can show that δ_c is the nearest singularity of θ determined as a radius of convergence limiting the convergence of the Taylor expansion of θ at $\delta = 0$. Several techniques have been developed to extract singularities from a finite number of Taylor series coefficients. The most commonly used are the Domb-Sykes plot ([14], [15]), Neville-Aitken extrapolation [15] and approximant methods, such as Padé approximants [15] and Hermite-Padé approximations ([10],[16],[17]), etc. The main tool used in this section is a simple method of series summation derived from the generalization of the Hermite-Padé approximants that can be summarized as follows:

Assuming that $U(\delta)$ is a local representation of an algebraic function obtained by a Taylor expansion in the given small parameter δ:

$$U_N(\delta) = \sum_{n=0}^{N} a_n \delta^n + O(\delta^{N+1}) \text{ as } \delta \to 0 \tag{11}$$

Herein we are concerned with the determination of the dominant behavior of the solution by using partial sum (11). Fuchs (cf. [15]) showed that the singularity must be either a pole or logarithmic branch. Therefore, $U(\delta)$ takes the form:

$$U(\delta) = \begin{cases} (\delta_c - \delta)^{\gamma} g(\delta) & \text{for } \gamma \neq 0, 1, 2, ... \\ (\delta_c - \delta)^{\gamma}\ ln|\delta_c - \delta| g(\delta) & \text{for } \gamma = 0, 1, 2, ... \end{cases} \tag{12}$$

where $g(\delta)$ is an analytic function and δ_c is the critical point with the exponent γ. A useful tool for extracting δ_c is the Hermit-Padé approximants, which are used in many branches of physics and applied mathematics to evaluate singularities of perturbation series.

Hermite-Padé approximation consists of finding polynomials P, Q, R of respective degrees p, q, r such that [17]:

$$P(\delta)U^1 + Q(\delta)U^2 + R(\delta)U^3 = O(\delta^{p+q+r}),\ \ P(0) = 1. \tag{13}$$

A particular case of such approximations are differential Hermite-Padé approximants obtained by taking:

$$U^1 = U,\ U^2 = DU,\ U^3 = D^2U \tag{14}$$

where D and D^2 are the differential operators given by $D = \frac{d}{d\delta}$, $D^2 = \frac{d^2}{d\delta^2}$.

In this work, we employ a special type of differential Hermite-Padé approximation technique ([10]), by rewriting the expression (13) in the form:

$$F_M(\delta, U_{N-1}) = 1 + A_{1N}(\delta)U^1 + A_{2N}(\delta)U^2 + A_{3N}(\delta)U^3 \tag{15}$$

such that

$$A_{iN}(\delta) = \sum_{j=1}^{M+i} \alpha_{ij}\delta^{j-1} \tag{16}$$

$$F_M(\delta, U) = O(\delta^{N+1})\text{as } : \delta \to 0 \tag{17}$$

where $M \geq 1$, $i = 1, 2, 3$. The unknowns coefficients α_{ij} depend only on the N given coefficients a_i and we shall take

$$N = 3(2 + M) \tag{18}$$

so that the number of equations equals the number of unknowns.

The dominant singularities of the branches of solutions of (11) are located at the zeros of A_{3N}, as shown by Della Dora and Di. Crescenzo [17]. The critical exponent γ_c can be obtained by using Newton's polygon algorithm and may be approximated by:

$$\gamma_c = 1 - \frac{A_{2N}(\delta_{cN})}{DA_{3N}(\delta_{cN})}. \tag{19}$$

5. Results and discussion

The maximum temperature θ_{max} is reached along the reacting slab centerline and is a characteristic quantity which qualifies the thermal stability. Thermal ignition criticality is governed by the values of the parameters δ_c and $\theta_c = \theta_{max}(\delta_c, \epsilon, m)$. In order to obtain these values, the Hermite-Padé approximation procedure described in section (4) above was applied to the first few terms of the Taylor series of the solution (10) of the boundary value problem (3-4). The results are shown in tables (1-4) below:

m	ϵ	δ_c	θ_c
-2,0,0.5	0	0.8784576579	1.119265476
- 2	0.01	0.9062277502	1.019446420
	0.1	0.9422258805	1.174428219
0	0.01	0.8878052761	1.120757730
	0.1	0.9882096285	1.221481288
0.5	0.01	0.8833192541	1.103164459
	0.1	0.9322155839	1.281171740

Table 1. Variation of δ_c and θ_c with respect to ϵ, when $\beta = 0$.

ϵ	δ_c	θ_c
0	0.8784575617	1.112480950
0.01	0.8877953343	1.120993488
0.05	0.9284003489	1.229733359
0.1	0.9882117413	1.39214472

Table 2: Computation showing criticality for Arrhenius reaction ($m = 0$) for different values of ϵ, when $\beta = 1$.

ϵ	M	δ_c	θ_c
0.01	2	0.8832992986	1.101141822
	3	0.8833200120	1.101342655
	4	0.8832854664	1.101007276
0.1	2	0.9322165287	1.262830935
	3	0.9322150065	1.262799659
	4	0.93221678454	1.262831870

Table 3: Computation showing the rapid convergence of criticality for bimolecular reaction ($m = 0.5$) for different values of ϵ, when $\beta = 1$.

ϵ	M	δ_c	θ_c
0.01	2	0.9062232837	1.135824308
	3	0.9062818966	1.136418609
	4	0.9062207229	1.135797806
0.1	2	1.313889395	2.020559500
	3	1.313889450	2.019024696
	4	1.313980247	2.020559500

Table 4: Computation showing the rapid convergence of criticality for sensitized reaction ($m = -2$) for different values of ϵ, when $\beta = 1$.

Tables 3-4 show the rapid convergence of the Hermite-Padé procedure to evaluate dominant singularity δ_c and crtical temperature θ_c with progressive increase in the number of series coefficients employed in the approximants.

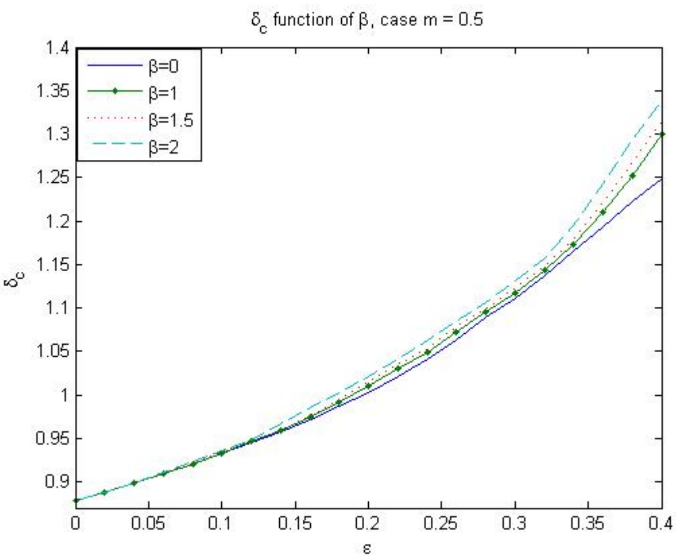

FIGURE 2. Variation of δ_c with dimensionless activation energy ϵ for various values of β. Case $m = 0.5$.

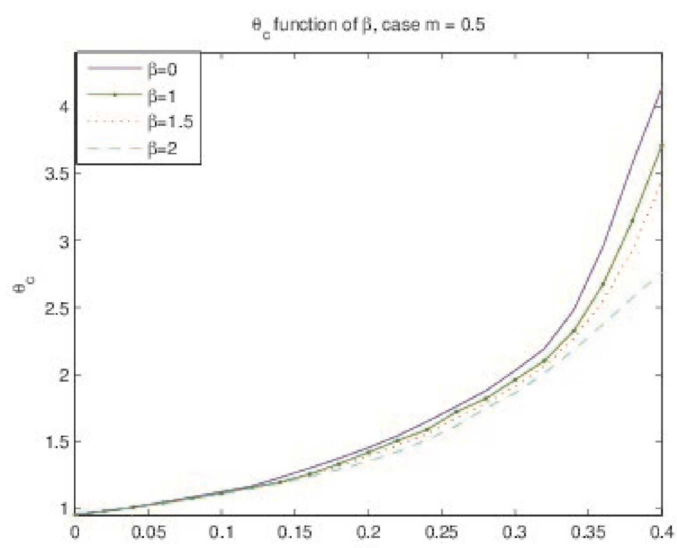

FIGURE 3. Variation of θ_c with dimensionless activation energy δ_c for various values of β. Case $m = 0.5$.

In the case of no heat exchange between the combustible material and the walls of the slab ($\beta = 0$), we get the critical values δ_c and θ_c, as shown in Table 1. We find that they are substantially equal to those calculated by other authors ([10],[11],[12]).

In the non-adiabatic case, i.e $\beta > 0$, Figures 2-3 show that as heat loss parameter β increases, critical ignition temperature θ_c decreases whereas critical Frank-Kamenetskii parameter δ_c increases for increasing values of ϵ. This leads to a delay in the development of thermal runaway in the reacting slab, due to an increase in the heat loss to the surrounding environment.

6. Conclusions

In this paper we applied the homotopy analysis method to solve a nonlinear boundary value problem arising from exothermic explosions. Furthermore, the obtained solutions are used to investigate thermal criticality by means of Hermite-Padé approach. The procedure shows the effect of heat loss parameter on the critical values of ignition temperature and on the Frank-Kamenetskii parameter.

The thermal runaway phenomena are investigated and the corresponding critical values are obtained through a bifurcation procedure. It is shown that an increase on the magnitude of the rate of heat transfer leads to an increase of thermal criticality as well as to a decrease of the maximum temperature. This enhances the thermal stability of the system.

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