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Thermal ignition in a reactive viscous plane-Poiseuille flow: a bifurcation study

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Thermal ignition for a reactive viscous flow between two symmetrically heated walls is investigated. The second order nonlinear boundary value problem governing the problem is obtained and solved analytically using a special type of Hermite-Padé approximation technique. We obtained very accurately the critical conditions for thermal ignition together with the two solution branches. It has been observed that an increase in viscous heating due to viscous dissipation can cause a rapid decrease in the magnitude of thermal ignition critical conditions.

Keywords: plane-Poiseuille flow, Hermite–Padé approximants, thermal ignition

1. Introduction

In chemical and petrochemical industries as well as petroleum refineries, the study of thermal explosion in a combustible reacting gas is of great important in order to ensure safety of life and properties. Hence, it is important to know the critical values of the basic physical quantities, such as the ambient temperature, surface characteristics, the chemistry of the reacting combustible gas and the physical storage geometry at which ignition occur. In a pioneering work, Frank–Kamenetskii (1955) derived a steady state mathematical model for thermal explosion process of a combustible material of constant density stored in between parallel heated walls using Arrhenius reaction rate with high activation energy approximation. He observed that there is no spontaneous thermal explosion if the channel width is less than a critical value determined by both the properties of the combustible reacting gas and the properties of exothermic chemical reaction. Thermal explosions occur when the reactions produce heat too rapidly for a stable balance between heat production and heat loss to be preserved. For detailed studies of thermal explosions, the reader might be referred to Aris [1], Boddington–Gray–Wake [3], Zaturska [18], Shonhiwa and Zaturska [13], Zeldovich et al. [19], Warnatz–Maas–Dibble [17], Taira [16], etc.,

In the present paper, we confine attention to steady developed flow between symmetrically heated walls. Our objective is to determine the critical conditions for thermal ignition as well bifurcation that takes place in the flow field using perturbation technique coupled with a special type of Hermite–Padé approximant. In the following sections, the problem is formulated, solved and discussed quantitatively.

2. Problem formulation

Consider a steady developed flow between symmetrically heated walls i.e. plane Poiseuille flow. The parabolic velocity profile in the streamwise direction is given $w = U(1 - y^2/a^2)$, where U is the mean velocity of the fluid. It is assumed that an exothermic chemical reaction occurs with Arrhenius dependence of the reaction rate on the temperature and large activation energy. The heat balance equation can be written as

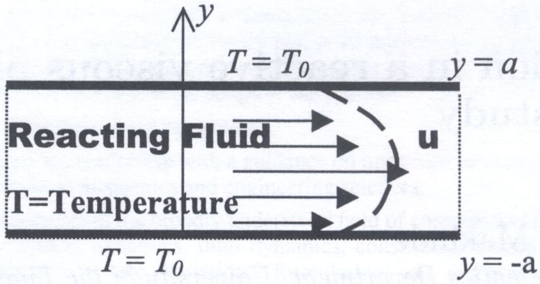

Fig. 1. Schematic diagram of the problem

$$\frac{\mathrm{d}^2T}{\mathrm{d}y^2} + \frac{Q\sigma(T_0)}{k}e^{-E/RT} + \frac{\mu}{k}\left(\frac{\mathrm{d}w}{\mathrm{d}y}\right)^2 = 0, \tag{1}$$

$$T(a) = T_0, \qquad \frac{\mathrm{d}T}{\mathrm{d}y}(0) = 0, \tag{2}$$

where T is the temperature of the reactive viscous fluid, y is the co-ordinate measured in the normal direction, k is the fluid thermal conductivity, μ is the fluid dynamic viscosity coefficient, Q is the thermal effect of the reaction, $\sigma\,(T_0)$ is the pre-exponential factor in the Arrhenius reaction rate that dependent on the wall reference temperature T_0, E is the activation energy and R is the universal gas constant. Introducing the following dimensionless variables;

$$u = \frac{(T-T_0)E}{RT_0^2}, \quad \eta = \frac{y}{a}, \quad \lambda = \frac{a^2Q\sigma(T_0)E}{RkT_0^2}e^{-E/RT_0},$$
$$\beta = \frac{4\mu U^2}{a^2Q\sigma(T_0)e^{-E/RT_0}}, \quad \frac{w}{U} = 1-\eta^2, \quad \varepsilon = \frac{RT_0}{E}, \tag{3}$$

we obtain

$$\frac{\mathrm{d}^2u}{\mathrm{d}\eta^2} + \lambda\left(e^{u/(1+\varepsilon u)} + \beta\eta^2\right) = 0, \tag{4}$$

$$\frac{\mathrm{d}u}{\mathrm{d}\eta}(0) = 0, \qquad u(1) = 0, \tag{5}$$

where β, λ and ε are the viscous heating parameter, the Frank–Kamenetskii parameter and the activation energy parameter respectively.

3. Solution method

To solve Eqs. (4)–(5), it is convenient to take a power series expansion in the Frank–Kamenetskii parameter λ, i.e.,

$$u = \sum_{i=0}^{\infty} u_i\lambda^i. \tag{6}$$

Substitute (6) into Eqs. (4)–(5) and collecting the coefficients of like powers of λ, with the computer aid such as MAPLE (Char et al. [4]), we obtained and solved the equations governing the first 22 coefficients of solution series (6). The solution for the temperature field is given as

$$u(\eta) = -\frac{\lambda}{12}(\eta^2-1)(\beta\eta^2+\beta+6) + \frac{\lambda^2}{360}(\eta^2-1)\left(\beta\eta^4+15\eta^2+\beta\eta^2-14\beta-75\right)+O(\lambda^3). \tag{7}$$

The rate of heat transfer across the wall is given as

$$H = -\frac{\mathrm{d}u}{\mathrm{d}\eta}(1) = \sum_{i=0}^{\infty} C_i\lambda^i = \lambda\left(1+\frac{\beta}{3}\right)+\lambda^2\left(\frac{1}{3}+\frac{\beta}{15}\right) + \lambda^3\left(\frac{1}{5}+\frac{16\beta}{315}+\frac{\beta^2}{405}-\frac{2\varepsilon}{15}-\frac{16\varepsilon\beta}{315}-\frac{2\varepsilon\beta^2}{405}\right)+O(\lambda^4). \tag{8}$$

We obtained the first 22 coefficients of series representing the wall heat flux (H) in Eq. (8) as shown in the Table 1 below

Table 1. Computation showing the coefficients of the wall heat flux (H) at very large activation energy ($\varepsilon = 0.0$)

i	C_i (β=0)	C_i (β=1)	C_i (β=5)	C_i (β=10)
0	0.00000000000	0.0000000000000	0.00000000000	0.000000000000
1	1.00000000000	1.3333333333333	2.66666666666	4.333333333333
2	0.33333333333	0.4000000000000	0.66666666666	1.000000000000
3	0.20000000000	0.2532627865961	0.51569664902	0.954850088183
4	0.14603174603	0.1965872810317	0.48503430725	1.068089112533
5	0.11816578483	0.1694696879010	0.50927341036	1.338092118484
6	0.10191438191	0.1558408133724	0.57147698061	1.794100946586
7	0.09181271403	0.1497495272531	0.67071894410	2.517326276415
8	0.08537598243	0.1485632254900	0.81314813588	3.649729163098
9	0.08132773378	0.1510033189886	1.01034038424	5.424236951455
10	0.07895434152	0.1564354509397	1.27976924770	8.219412315014
11	0.07783241005	0.1645728448385	1.64639586969	12.65091819853
12	0.07770055641	0.1753396095686	2.14527175466	19.72323433488
13	0.07839392514	0.1888040113777	2.82536468870	31.08138209782
14	0.07980851209	0.2051455904644	3.75502835532	49.42945951523
15	0.08188070824	0.2246402395754	5.02976019330	79.22823097161
16	0.08457509081	0.2476557815904	6.78318438313	127.8606445848
17	0.08787691574	0.2746543944672	9.20260340645	207.5836388981
18	0.09178741234	0.3062000922292	12.5510379386	338.8037793750
19	0.09632081711	0.3429704487541	17.1984970268	555.5858187505
20	0.10150253016	0.3857723098850	23.6663965504	914.9340265611
21	0.10736802463	0.4355615927447	32.6907285469	1512.458330982

4. Bifurcation study

The main tool of this paper is a simple technique of series summation based on the generalization of Padé approximants and may be described as follows. Let us suppose that the partial sum

$$U_{N-1}(\lambda)=\sum_{i=0}^{N-1} a_i\lambda^i = U(\lambda)+O(\lambda^N) \quad \text{as} \quad \lambda\to 0, \tag{9}$$

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 (9). We expect that the accuracy of the critical parameters will ensure the accuracy of the solution, Makinde [11]. It is well known that the dominant behaviour of a solution of a linear ordinary differential equation can often be written as Guttmann [6],

$$U(\lambda)\approx\begin{cases} K(\lambda_c-\lambda)^{\alpha} & \text{for} \quad \alpha\neq 0,1,2,\ldots \\ K(\lambda_c-\lambda)^{\alpha}\ln|\lambda_c-\lambda & \text{for} \quad \alpha\neq 0,1,2,\ldots \end{cases} \quad \text{as} \quad \lambda\to\lambda_c \tag{10}$$

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 context 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

$$F_d(\lambda,U_{N-1})=A_{0N}(\lambda)+A^d_{1N}(\lambda)U^{(1)}+A^d_{2N}(\lambda)U^{(2)}+A^d_{3N}(\lambda)U^{(3)}, \tag{11}$$

such that

$$A_{0N}(\lambda)=1, \qquad A_{iN}(\lambda)=\sum_{j=1}^{d+i} b_{ij}\lambda^{j-1}, \tag{12}$$

and

$$F_d(\lambda,U)=O(\lambda^{N+1}) \quad \text{as} \quad \lambda\to 0, \tag{13}$$

where $d\geq 1$, $i=1, 2, 3$. The condition (12) 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 (11). The requirement (13) 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

$$N=3(2+d), \tag{14}$$

so that the number of equations equals the number of unknowns. Equation (13) is a new special type of Hermite–Padé approximants. Both the algebraic and differential approximants form of Eq. (13) are considered. For instance, we let

$$U^{(1)}=U, \qquad U^{(2)}=U^2, \qquad U^{(3)}=U^3, \tag{15}$$

and obtain a cubic Padé approximant. This gives an extension of the idea of quadratic Padé approximants by Shafer [12] and Sergeyev [14]. For the above cubic algebraic approximants, a simple turning point occurs where

$$F_d(\lambda,U)=0 \quad \text{and} \quad \frac{\mathrm{d}F_d(\lambda,U)}{\mathrm{d}U}=0. \tag{16}$$

Furthermore, Drazin and Tourigny [5], Sergeyev and Goodson [15], Makinde [10] had also suggested a similar form of higher order algebraic approximants. Generally, 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

$$U^{(1)} = U, \qquad U^{(2)} = DU, \qquad U^{(3)} = D^2U, \tag{17}$$

in Eq. (12), where D is the differential operator given by $D = \mathrm{d}/\mathrm{d}\lambda$. This leads to a second order differential approximants. It is an extension of the integral approximants idea by Hunter and Baker [8] and enables us to obtain the dominant singularity in the flow field i.e. by equating the coefficient $A_{3N}(\lambda)$ in the Eq. (13) to zero. 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 that are structurally stable are simple turning points. Hence, in practice, one almost invariably obtains $\alpha_N = 1/2$. If we assume a singularity of algebraic type as in Eq. (10), then the exponent may be approximated by

$$\alpha_N = 1 - \frac{A_{2N}(\lambda_{CN})}{DA_{3N}(\lambda_{CN})}. \tag{18}$$

Using the above procedure, we performed series summation, improvement and bifurcation study on the solution series obtained in Table 1. Our results show the dominant singularity in the problem to be $\lambda_c(\beta, \varepsilon)$ with the critical exponent $\alpha_c = 0.5$ and maximum fluid temperature ($u_{\max}$ i.e. at $y = 0$) as shown in the Table 2 below

Table 2. Computations showing the procedure rapid convergence for $\varepsilon = 0.0$ and $\beta = 0.0$

d	N	$u_{\max}$	$\lambda_c(\beta=0)$	α_c
1	9	1.18701002044	0.878451473	0.499919
2	12	1.18684567133	0.878457670	0.499999
3	15	1.18684216116	0.878457679	0.499999
4	18	1.18684216863	0.878457679	0.500000
5	21	1.18684216863	0.878457679	0.500000

5. Graphical results and discussion

Figure 2 shows the temperature distribution of the reactive viscous fluid. Generally, a parabolic profile is observed with maximum temperature along the centerline of the channel. It is noteworthy that an increase in the Frank–Kamenetskii parameter (λ) due to continuous exothermic chemical reaction will facilitate a gradual increase in the reactive fluid temperature. Similar effect is observed with an increase in the viscous heating parameter due to energy dissipation as shown in Fig. 3. The rapid convergence of our procedure in Sec. 4 is demonstrated in Table 2 with increasing number of terms of the solution series utilized. We obtained very accurately the magnitude of critical conditions for thermal ignition $\lambda_c(\beta,\varepsilon)$ as shown in Table 3. It is interesting to note that $\lambda_c \rightarrow 0$ as $\beta \rightarrow \infty$ at a given large activation energy ($0 \leq \varepsilon \ll 1$).This implies that additional heating due to viscous dissipation can facilitate early occurrence of thermal ignition by increasing the reactive fluid temperature. Meanwhile, a decrease in fluid activation energy ($\varepsilon = 0.1$) may increase the magnitude of thermal criticality; hence causes delay in the occurrence of thermal ignition. For the case of a stationary reactive fluid (i.e. $\beta = 0$), our result for critical conditions for thermal ignition represents a great improvement on Frank–Kamenetskii (1955) who obtained $\lambda_c(\beta=0) = 0.88$. Furthermore, it is interesting to note that λ_c represents a simple turning point with critical exponent $\alpha_c = 0.5$

Table 3. Computations showing thermal criticality for various values of parameters (β, ϵ)

ε	β	$u_{\max}$	λ_c	α_c
0.1	1.0	1.62681183925	0.93301095	0.5000000
0.1	5.0	1.95575679764	0.78151707	0.5000000
0.0	0.0	1.18684216863	0.87845767	0.5000000
0.0	1.0	1.25409582662	0.82295379	0.5000000
0.0	5.0	1.46185090079	0.67257689	0.5000000
0.0	10.0	1.64665791280	0.56195708	0.5000000

(i.e a link between two solution branches). A sketch of bifurcation diagram for the heat flux at the wall is shown in Fig. 4, the presence of two solution branches (i.e. types I and II) within the region $0 < \lambda < \lambda_c$ and above which no real solution of a given type is observed (i.e. $\lambda > \lambda_c$). Finally, in this paper, we have utilized a special type of Hermite–Padé approximant to investigate the bifurcation and critical conditions for thermal explosions. The chief novelty of this procedure is its ability to reveal the dominant singularities together with solution branches of the underlying nonlinear problem in addition to the branch represented locally by the original series. Generally, we have found that this new method is very competitive and enhanced the analytic continuation of a given solution series beyond its radius of convergence.

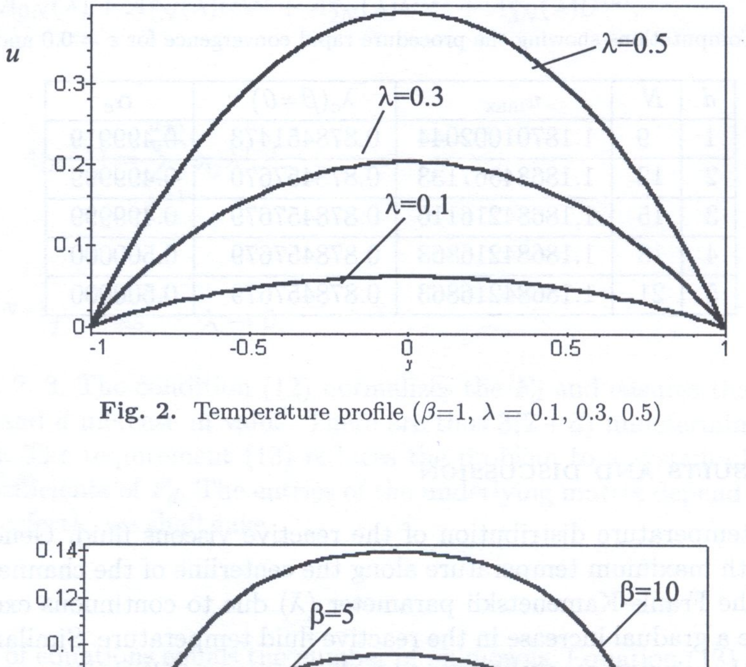

Fig. 2. Temperature profile (β=1, λ = 0.1, 0.3, 0.5)

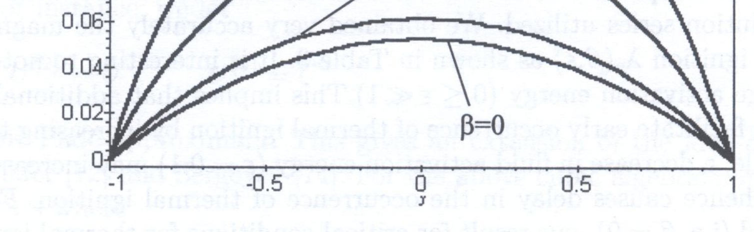

Fig. 3. Temperature profile (λ = 0.1, β = 0, 1, 5, 10)

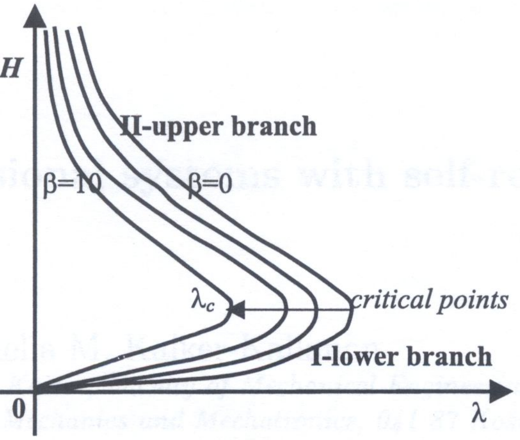

Fig. 4. A sketch of bifurcation diagram for the problem

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