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Critical parameters for some non-Class A configurations in combustion theory, with non-uniform boundary temperatures

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Abstract. The critical parameters for a problem in combustion theory for certain non-Class A geometries are computed using a transcendental equation derived from the non-linear parabolic equation. When possible, results are compared with existing ones in the literature.

1. Introduction

A simple model governing the combustion of a material can be formulated in non-dimensional form as follows:

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta + \delta \exp\left(\frac{\alpha\theta}{\alpha + \theta}\right); \quad t > 0, \mathbf{x} \in D. \tag{1.1}$$

Here, θ is the temperature, $\mathbf{x}$ and t are respectively the spatial and time variables, and δ, α are positive parameters. Analytical studies of the equation have been confined mainly to the so-called Class A geometries, viz. the domain D is an infinite slab, an infinite circular cylinder, or a sphere. The initial condition for (1.1) is usually taken as $\theta(\mathbf{x}, 0) = 0$, and the boundary condition taken as $\theta = 0$. The natural boundary condition $\partial\theta/\partial\nu + \beta\theta = 0$, where ν is in the direction of the outward normal to D and β is the Biot number, has also been considered. In these studies, a quantity of primary interest is the critical value of δ, δ_{cr}, through which the solution of (1.1) undergoes a rapid transition from being $O(1)$ to $O(e^{\alpha})$, when $\alpha \gg 1$. Such a situation is referred to as thermal explosion. Another quantity of interest is the transitional value of α, α_{tr}, below which (1.1) loses the abrupt change in its response to a change in δ. Such a situation is referred to as loss of criticality. (See [1, 2, 3], among others.)

When δ is below the critical value, the solution of (1.1), for $\alpha \gg 1$, can still become exponentially large if the initial and/or the boundary conditions are sufficiently large. The influence of the initial and boundary conditions has been considered by Tam in [5] and [6] and by Tam and Chapman [7]. Recently, using a comparison result for parabolic equations, and a two-step linearization, Tam [8] showed that the influence of the initial and boundary conditions can be examined in terms of the solution of the simple heat equation and the first eigenfunction for the domain. Estimates of the critical parameters are given by the solution of a relatively simple transcendental equation. The need to solve the original non-linear parabolic equation is obviated.

In this note, we consider a rectangular block and a finite circular cylinder. The influence of the Biot number on δ_{cr} and α_{tr} is examined in Section 2, while the influence of a simple non-uniform boundary condition on δ_{cr} is examined in Section 3. In a numerical study of (1.1) subject to $\theta(\mathbf{x}, 0) = 0$, $\theta = 0$ on ∂D, Parks [4] obtained δ_{cr} for a cube and a right circular cylinder. Since $\theta = 0$ on ∂D can be considered as the limiting situation as $\beta \to \infty$ in the natural boundary condition, we compare these values with the estimates obtained here. It is seen that good agreement is achieved.

2. The critical parameters for a rectangular block and a finite circular cylinder, with natural boundary conditions

We consider the following initial and boundary conditions for the solution of (1.1):

$$\theta(\mathbf{x}, 0) = 0, \quad \frac{\partial \theta}{\partial \nu} + \beta\theta = 0 \quad \text{for} \quad \mathbf{x} \in \partial D,$$

and we want to obtain estimates of the transitional value of α; and critical values of δ, for given values of α and β.

For the sake of completeness, we include the following discussions leading to the transcendental equation which will be used to obtain estimates on δ_{cr} and α_{tr}. Further details can be found in [8].

Let ϕ_n and λ_n^2 be the normalized eigenfunctions and eigenvalues of the boundary-value problem

$$\nabla^2\phi_n = -\lambda_n^2\phi_n,$$

$$\frac{\partial \phi_n}{\partial \nu} + \beta\phi_n = 0 \quad \text{on} \quad \partial D. \tag{2.1}$$

Without loss of generality, we can take $\phi_1 > 0$. Let $T(t)$ be the solution of the initial-value problem

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -\lambda_1^2 T + \delta \int_D \phi_1(\xi) \exp\left\{\frac{\alpha T\phi_1(\xi)}{\alpha + T\phi_1(\xi)}\right\} \mathrm{d}V, \quad T(0) = 0. \tag{2.2}$$

Equivalently, T can be expressed as the solution of the integral equation

$$T = \delta \mathrm{e}^{-\lambda_1^2 t} \int_0^t \mathrm{e}^{\lambda_1^2 \tau}\phi_1(\xi) \cdot \exp\left\{\frac{\alpha T(\tau)\phi_1(\xi)}{\alpha + T(\tau)\phi_1(\xi)}\right\} \mathrm{d}\tau \tag{2.3}$$

where the dot is used to denote the inner product $f \cdot g = \int_D f(\xi) g(\xi)\,\mathrm{d}V$. With T given by the above, we consider the IBVP

$$\chi_t = \nabla^2\chi + \delta \exp\left\{\frac{\alpha m(\mathbf{x})\, T(t)\, \phi_1(\mathbf{x})}{\alpha + m(\mathbf{x})\, T(t)\, \phi_1(\mathbf{x})}\right\}, \tag{2.4}$$

$$\chi(\mathbf{x}, 0) = 0; \quad \frac{\partial \chi}{\partial \nu} + \beta \chi = 0, \quad \mathbf{x} \text{ on } \partial D;$$

where $m(\mathbf{x}) > 0$ is a function to be determined.

Let $K(\mathbf{x}, \boldsymbol{\xi}, t)$ be the Robin function for the system

$$K_t - \nabla^2 K = 0,$$

$$K(\mathbf{x}, \boldsymbol{\xi}, 0) = 0; \quad \frac{\partial K}{\partial \nu} + \beta K = 0, \quad \mathbf{x} \text{ on } \partial D.$$

We have

$$K(\mathbf{x}, \boldsymbol{\xi}, t) = \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n^2 t} \phi_n(\mathbf{x}) \phi_n(\boldsymbol{\xi}).$$

Since K is the response function to a point source, it is clear that $K > 0$ in D. The solution of (2.4) can be written as

$$\chi(\mathbf{x}, t; m) = \delta \int_0^t K(\mathbf{x}, \boldsymbol{\xi}, t - \tau) \cdot \exp \left\{ \frac{\alpha m(\boldsymbol{\xi}) T(\tau) \phi_1(\boldsymbol{\xi})}{\alpha + m(\boldsymbol{\xi}) T(\tau) \phi_1(\boldsymbol{\xi})} \right\} \mathrm{d}\tau. \tag{2.5}$$

Our objective is to choose $m(\mathbf{x})$ so that $\chi(\mathbf{x}, t)$ is a lower solution of (1.1), subject to $\theta(\mathbf{x}, 0) = 0$, $\partial\theta/\partial\nu + \beta\theta = 0$ on ∂D; i.e., we wish to make

$$P\chi = \chi_t - \nabla^2 \chi - \delta \exp\left(\frac{\alpha\chi}{\alpha + \chi}\right) \leqslant 0,$$

which then implies $\chi(\mathbf{x}, t; m) \leqslant \theta$. Now, we have

$$P\chi = \delta \left\{ \exp\left[\frac{\alpha m T \phi_1}{\alpha + m T \phi_1}\right] - \exp\left[\frac{\alpha\chi}{\alpha + \chi}\right] \right\}.$$

Since the function $\exp[\alpha u/(\alpha + u)]$ is an increasing function of u, we will have $P\chi \leqslant 0$, if we can choose m to make

$$m T \phi_1 \leqslant \int_0^t K(\mathbf{x}, \boldsymbol{\xi}, t - \tau) \cdot \exp\left[\frac{\alpha m T \phi_1}{\alpha + m T \phi_1}\right] \mathrm{d}\tau. \tag{2.6}$$

Using (2.3), the above becomes

$$m \int_0^t \mathrm{e}^{-\lambda_1^2 (t - \tau)} \phi_1(\mathbf{x}) \phi_1(\boldsymbol{\xi}) \cdot \exp\left[\frac{\alpha T(\tau) \phi_1(\boldsymbol{\xi})}{\alpha + T(\tau) \phi_1(\boldsymbol{\xi})}\right] \mathrm{d}\tau$$

$$\leqslant \int_0^t K(\mathbf{x}, \boldsymbol{\xi}, t - \tau) \cdot \exp\left[\frac{\alpha m(\boldsymbol{\xi}) T(\tau) \phi_1(\boldsymbol{\xi})}{\alpha + m(\boldsymbol{\xi}) T(\tau) \phi_1(\boldsymbol{\xi})}\right] \mathrm{d}\tau. \tag{2.7}$$

Since the exponential function in the integrands is bounded between 1 and exp (α), and both ϕ_1 and K are positive in D, it is clear that by choosing m to be sufficiently small, the above inequality can be satisfied, and consequently, we have constructed a lower solution for θ. An entirely analogous procedure with $M > 0$ replacing m yields an upper solution if M is sufficiently large, i.e., $\chi(\mathbf{x}, t; M) > \theta$. If m and M do not deviate much from unity, $\chi(\mathbf{x}, t; 1)$ serves as a good approximation for θ. Numerical work on a specific example in [8] showed that the derivation of m and M from unity is indded small. Further, by examining (2.7), we see that the deviation is governed by the magnitude of

$$\left\{\sum_{n=2}^{\infty} \mathrm{e}^{-\lambda_n^2(t-\tau)} \phi_n(\mathbf{x}) \phi_n(\xi)\right\} \cdot \exp\left\{\frac{\alpha T(\tau) \phi_1(\xi)}{\alpha + T(\tau) \phi_1(\xi)}\right). \tag{2.8}$$

Since the shape of the exponential function in (2.8) is close to a constant multiple of ϕ_1, the orthogonality of the eigenfunctions implies that expression (2.8) is small. On the basis of the above observations, we shall take $\chi(\mathbf{x}, t; 1)$ as an approximation for θ.

We now make the following observation. The function $\chi(\mathbf{x}, t; 1)$ increases with $T(t)$. If $T(t)$ remains O(1), so does χ. If $T(t)$ becomes exponentially large, χ will be exponentially large also. Thus, the behaviour of T determines that of χ. To see the influence of α and δ on T, we need only examine the transcendental equation

$$\frac{\lambda_1^2 T}{\delta} = \int_D \phi_1(\xi) \exp\left[\frac{\alpha T \phi_1(\xi)}{\alpha + T\phi_1(\xi)}\right] \mathrm{d}V, \tag{2.9}$$

which gives the stationary values of T. The integral in (2.9), plotted against T, is an S-shaped curve. If δ is small, (2.9) has a unique solution which is O(1). If δ increased past a certain value δe, (2.9) has three solutions, the small one is O(1) while the large one is O(e^{α}). Thus, if α is sufficiently large, the large solution is exponentially large. If δ is further increased past the critical value, δ_{cr}, (2.9) again has only one solution, which is O(e^{α}). Regarding the dependence of the solution on α, we note that if the value of α is decreased from $\alpha \gg 1$, we reach a transitional value α_{tr}, at which point the S-shaped curve flattens out so that (2.9) has only one solution regardless of the magnitude of δ. This phenomenon is referred to as the loss of criticality. We now apply (2.9) to the following specific configurations:

2.1. The rectangular block

We consider the rectangular block D defined by $-1 \leqslant x \leqslant 1$, $-a \leqslant y \leqslant a$, $-b \leqslant z \leqslant b$. In a straight-forward manner, we obtain the first eigenvalue for (2.1):

$$\lambda_1^2 = k_1^2 + l_1^2 + \gamma_1^2,$$

where k_1, l_1 and γ_1 are respectively the first positive zeroes of the equations $k \tan k = \beta$; $l \tan la = \beta$ and $\gamma \tan \gamma b = \beta$. The corresponding normalized eigenfunction is

$$\phi_1 = K \cos k_1 x \cos l_1 y \cos \gamma_1 z$$

Table 1. δ_{cr} for different values of α and β for the rectangular block $-1 \leqslant x \leqslant 1$, $-1 \leqslant y \leqslant 1$, $-b \leqslant z \leqslant b$

α	δ_{cr}		$\beta = 10000$	
	$b = 1$		$b = 2$	$b = 4$
20	2.604	2.68*	1.953	1.790
60	2.499	2.58*	1.953	1.717
100	2.477	2.53*	1.858	1.703

* From Parks [4], $\beta \to \infty$

α	δ_{cr}	$\beta = 100$	
	$b = 1$	$b = 2$	$b = 4$
20	2.554	1.917	1.756
60	2.499	1.838	1.684
100	2.429	1.824	1.671

α	δ_{cr}	$\beta = 10$	
	$b = 1$	$b = 2$	$b = 4$
20	2.175	1.645	1.498
60	2.087	1.578	1.437
100	2.070	1.566	1.425

Table 2. α_{tr} for different values of β for the rectangular block $-1 \leqslant x \leqslant 1$, $-1 \leqslant y \leqslant 1$, $-b \leqslant z \leqslant b$

b	α_{tr}		
	$\beta = 10$	$\beta = 100$	$\beta = 10000$
1	4.193	4.209	4.209
2	4.179	4.209	4.209
3	4.198	4.209	4.209

where

$$K = \left(1 + \frac{\sin 2k_1}{2k_1}\right)^{-1/2}\left(a + \frac{\sin 2al_1}{2l_1}\right)^{-1/2}\left(b + \frac{\sin 2b\gamma_1}{2\gamma_1}\right)^{-1/2}.$$

For various values of a, b, β, we compute the values of δ_{cr}. Some representative results are tabulated in Table 1, and compared with existing results when available. The transitional values α_{tr} are also computed and tabulated in Table 2.

2.2. *The finite circular cylinder*

We consider a circular cylinder D defined by $0 \leqslant r \leqslant 1$, $-b \leqslant z \leqslant b$. We obtained the first eigenvalue for (2.1):

$$\lambda_1^2 = \mu_1^2 + \gamma_1^2$$

where γ_1 is as determined in the last section, and μ_1 is the first zero of the equation

$$\mu J_1(\mu) = \beta J_0(\mu),$$

Table 3. δ_{cr} for different values of β, $\alpha = 20$, for the finite circular cylinder $0 \leqslant r \leqslant 1$, $-b \leqslant z \leqslant b$

b	δ_{cr}			
	$\beta = 10$	$\beta = 100$	$\beta = 10000$	$\beta \to \infty$, Parks
1	2.568	2.661	2.912	2.93
2	2.547	2.801	2.259	
4	2.506	2.979	2.096	

Table 4. α_{tr} for different values of β for the finite circular cylinder $0 \leqslant r \leqslant 1$, $-b \leqslant z \leqslant b$

b	α_{tr}		
	$\beta = 10$	$\beta = 100$	$\beta = 10000$
1	4.1836	4.1992	4.2070
2	4.1914	4.1992	4.1992
4	4.1914	4.1992	4.1992

where J_0 and J_1 are respectively Bessel functions of order zero and one. The corresponding normalized eigenfunction is

$$\phi_1 = K \cos \gamma_1 z J_0(\mu r)$$

where

$$K = \sqrt{\frac{1}{\pi}} \left(b + \frac{\sin 2b\gamma_1}{2\gamma_1} \right)^{-1/2} (\mu_1^2 + \beta^2)^{-1/2} \frac{\mu_1}{J_0(\mu_1)}.$$

As in the previous section, we tabulate some critical values of δ in Table 3, and the transitional value of α in Table 4.

3. The critical parameters for a rectangular block and a finite circular cylinder, with non-uniform boundary conditions

We consider the following initial and boundary conditions for the solution of (1.1):

$$\theta(\mathbf{x}, 0) = 0; \quad \theta(\mathbf{x}, t) = g(\mathbf{x}), \quad \mathbf{x} \in \partial D. \tag{3.1}$$

Let ϕ_1 and λ_1 denote respectively the first eigenvalue and eigenfunction of the problem

$$\nabla^2 \phi = -\lambda^2 \phi,$$

$$\phi = 0 \text{ on } \partial D; \tag{3.2}$$

and let $P(\mathbf{x}, t)$ be the solution of

$$P_t = \nabla^2 P,$$

$$P(\mathbf{x}, 0) = 0; \quad P(\mathbf{x}, t) = g(\mathbf{x}) \text{ on } \partial D. \tag{3.3}$$

In almost the same way that we obtained (2.9), we have, from [8], the following transcendental equation

$$\frac{\lambda_1^2 T}{\delta} = \int_D \phi_1(\xi) \exp\left[\frac{\alpha(T\phi_1(\xi) + P(\xi, \infty))}{\alpha + T\phi_1(\xi) + P(\xi, \infty)}\right] \mathrm{d}V. \tag{3.4}$$

For a given $g(\mathbf{x})$, and hence $P(\xi, \infty)$, a critical value δ_{cr} can be determined such that for $\delta > \delta_{cr}$, (3.4) has only one solution which is $O(e^{\alpha})$. We apply this result to the two configurations considered in Section 2, with a simple non-uniform boundary temperature.

3.1. The rectangular block

We let D be defined by $0 \leqslant x \leqslant 1$, $0 \leqslant y \leqslant a$, $0 \leqslant z \leqslant b$; and $g(\mathbf{x})$ be given by

$$g(0, y, z) = A \sin\frac{\pi y}{a} \sin\frac{\pi z}{b},$$

$$g = 0 \text{ on all other bounding surfaces.}$$

We then have

$$\lambda_1^2 = \left(1 + \frac{1}{a^2} + \frac{1}{b^2}\right)\pi^2,$$

$$\phi_1 = \frac{2\sqrt{2}}{\sqrt{ab}} \sin \pi x \sin\frac{\pi y}{a} \sin\frac{\pi z}{b}$$

and

$$P(\mathbf{x}, \infty) = \frac{A \sin\frac{\pi y}{a} \sin\frac{\pi z}{b}}{\sinh\left[\frac{\pi(a^2 + b^2)^{1/2}}{ab}\right]} \sinh\left[\frac{\pi(a^2 + b^2)^{1/2}}{ab}(1 - x)\right].$$

For different values of a, b and A, we compute the value of δ_{cr} for $\alpha = 20$. The results are given in Table 5.

Table 5. δ_{cr} for various values of A, $\alpha = 20$, for the rectangular block $0 \leqslant x \leqslant 1$, $0 \leqslant y \leqslant 1$, $0 \leqslant z \leqslant 1$ with $\theta(0, y, z) = A \sin \pi y \sin \pi z$, $\theta = 0$ on all other sides

A	0	5	10	20	40
δ_{cr}	10.418	5.868	2.655	0.4596	0.03599
δ_{cr} adjusted to scaling of Sec. 2	2.604 (Parks' value = 2.68)	1.467	0.664	0.115	0.09000

Table 6. δ_{cr} for various values of A, $\alpha = 20$, for the circular cylinder $0 \leqslant r \leqslant 1$, $0 \leqslant z \leqslant a$, with $\theta(0, r) = AJ_0(2.405r)$; $\theta = 0$ on all other sides

A	0	5	10	20	40
δ_{cr} $a = 1$	5.526	1.900	0.585	0.730	0.00513
δ_{cr} $a = 2$	2.913 (Parks' value = 2.93)	1.736	0.827	0.150	0.01200

3.2. *The finite circular cylinder*

We let D be defined by $0 \leqslant r \leqslant 1$, $0 \leqslant z \leqslant a$; and $g(\mathbf{x})$ be given by

$$g(r, 0) = AJ_0(cr), \quad c = 2.405,$$

$$g(r, z) = 0 \text{ on all other bounding surfaces.}$$

We then have

$$\lambda_1^2 = c^2 + \frac{\pi^2}{a^2},$$

$$\phi_1 = \sqrt{\frac{2}{a\pi}}\,\frac{1}{0.5191}\sin\frac{\pi z}{a}\,J_0(cr)$$

and

$$P(r, z, \infty) = \frac{A}{\sinh ca}\sinh c(a - z)\,J_0(cr).$$

For different values of a and A, we compute the value of δ_{cr} for $\alpha = 20$ and the results are given in Table 6.

4. Concluding remarks

We have shown that for non-Class A geometries where the first eigenfunction can be found, the critical parameters for the non-linear parabolic equation can be estimated relatively easily. Even for other geometries where the first eigenfunction cannot be determined analytically, using the transcendental equation to estimate the critical parameters can still offer some computational advantage. Further, the two-step linearization procedure can conceivably be used in similar problems.

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