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COMPUTATION OF CRITICAL PARAMETERS FOR A PROBLEM IN COMBUSTION THEORY

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Abstract

An iteration scheme previously obtained by the author is used to study the dependence of criticality on initial data and the parameters in a combustion problem. Numerical results are presented for a slab, a cylinder and a sphere. These are compared with the results of previous workers.

1. Introduction

A central equation in the study of auto-catalytic reactions is

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta + \delta F(\theta) \quad \text{in } D,$$

subject to

$$\theta(\mathbf{x}, 0) = h(\mathbf{x}); \qquad \theta = 0 \text{ on } \partial D,$$

where $F(\theta) = \exp(\alpha\theta/(\alpha + \theta))$, θ is the temperature, x, t are the spatial and time variables respectively and δ and α are positive parameters.

Recently, Tam [3], [4] considered the role of the initial data in a problem in combustion theory, for the special geometries of an infinite slab, an infinite circular cylinder, and a sphere; and the disappearance of criticality was examined using the upper and lower solutions constructed in [5].

In this note, we use the iteration scheme obtained in [3] and [4] to study more extensively the dependence of criticality on the initial data as well as the

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parameters. Since the treatment is numerical, some of the approximations used in [3] and [4] in order to give analytic results are obviated. The improvement thus achieved is especially significant when α is close to 4. In the next section, we quote the iteration scheme, then we present the numerical results in tables for the case of the slab, the cylinder and the sphere.

2. Criticality dependence on initial data and parameters

We have from [3] and [4] the result

$$\theta_{n+1}(r, t) \sim \delta u_1(r) \int_T^t \exp[-\lambda_1^2(t-s)] u_1(\xi) \cdot F(\theta_n(\xi, s))\, ds$$

where r denotes the only spatial variable, λ_1^2 and $u_1(r)$ the first eigenvalue and normalized eigenfunction of the eigenvalue problem

$$\nabla^2 u_k + \lambda_k^2 u_k = 0$$
$$u_k = 0 \qquad \text{on } \partial D,$$

and

$$u_1(\xi) \cdot F(\theta_n(\xi, s)) = \int_D u_1(\xi) F(\theta_{n+1}(\xi, s))\, d\xi,$$

with D denoting the region under consideration. If, for $t > T$, we have $u_1(\xi) \cdot F(\theta_n(\xi, s)) \sim K_n$ for some n, where K_n is independent of s, then for $t \gg T$ we have

$$\theta_{n+1}(r, t) \sim \frac{K_n \delta}{\lambda_1^2} u_1(r).$$

Using the above, we consider, for s large,

$$u_1(\xi) \cdot F(\theta_n(\xi, s)) \sim K_{n+1},$$

and from which we have, for t large,

$$\theta_{n+2}(r, t) \sim \frac{K_{n+1}\delta}{\lambda_1^2} u_1(r).$$

Thus, the steady state reached is deduced by comparing K_{n+1} with K_n. In [3] and [4] we made approximations in the evaluation of K_{n+1}. In this note, we obtain K_{n+1} numerically, from which we determine all other critical parameters. Criticality disappears when $\alpha < \tilde{\alpha}$, which depends on geometry, but in all cases is slightly larger than 4. When $\alpha > \tilde{\alpha}$, there is a unique steady state when $\delta < \delta_e(\alpha)$ or when $\delta > \delta_{cr}(\alpha)$. For $\delta_e < \delta < \delta_{cr}$, there are two stable steady states, the one with the larger maximum referred to as super-critical, and the one with the smaller maximum referred to as sub-critical. In this range, we determine $v^*(\delta, \alpha)$ such that for $K_n > \delta^{-1}v^*$, the super-critical state is reached while for $K_n < \delta^{-1}v^*$, the sub-critical state is reached. The limiting values of K_n, namely $\bar{K}_\infty$ and $\tilde{K}_\infty$ are also determined. These quantities are presented in tables.

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TABLE 1

Values of $\tilde{K}_\infty$, and $\bar{K}_\infty$ for some values of α and δ for the slab.

α	δ	$\tilde{K}_\infty$	v^*	$\bar{K}_\infty$
100	$\delta_e = 1.02E-38$	$.920E-38$	83260	83260
	0.1	0.091	54.0	$0.243E43$
	1.0	1.01	29.5	$0.242E44$
	2.0	2.35	20.9	$0.484E44$
	$\delta_{cr} = 3.546$	8.51	8.51	$0.858E44$
70	$\delta_e = 5.33E-26$	$0.48E-25$	40429	40429
	0.1	0.091	56.2	$0.2265E30$
	1.0	1.01	30.3	$0.226E31$
	2.0	2.35	21.3	$0.4529E31$
	$\delta_{cr} = 3.5633$	8.61	8.61	$0.806E31$
40	$\delta_e = 1.837E-13$	$0.1656E-12$	12892	12892
	0.1	0.09	62.2	$0.212E17$
	1.0	1.01	32.2	$0.2119E18$
	2.0	2.35	22.4	$0.4238E18$
	$\delta_{cr} = 3.6$	8.81	8.81	$0.764E18$
20	$\delta_e = 2.164E-5$	$0.1948E-4$	3039	3039
	0.1	0.91	84.0	$0.4367E8$
	1.0	1.01	37.9	$0.4368E9$
	2.0	2.34	25.5	$0.8790E9$
	$\delta_{cr} = 3.708$	9.34	9.34	$0.162E10$
15	$\delta_e = 1.77E-3$	$0.1593E-2$	1639	1639
	0.5	0.475	59.6	$0.1469E7$
	1.6	1.75	33.1	$0.4706E7$
	2.5	3.22	23.3	$0.7355E7$
	$\delta_{cr} = 3.77$	9.74	9.74	$0.11E8$
8	$\delta_e = 0.51$	0.4846	390	390
	1.0	1.01	96.6	1970
	2.0	2.33	46.8	4678
	3.0	4.25	28.5	7366
	$\delta_{cr} = 4.06$	11.6	11.6	10220
4.5	$\delta_e = 4.457$	9.875	73	73
	4.7	12.52	35.15	126
	$\delta_{cr} = 4.88$	19.8	19.8	148
$\tilde{\alpha} = 4.069$	$\delta_e = 5.227 = \delta_{cr}$	34	34	34

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TABLE 2

Values of $\tilde{K}_\infty$, v^*, and $\bar{K}_\infty$ for some values of α and δ for a sphere.

α	δ	$\tilde{K}_\infty$	v^*	$\bar{K}_\infty$
100	$\delta_e = 1.08E-38$	$0.1685E-37$	138080	138080
	0.1	0.161	74.19	$0.429E43$
	1.0	1.79	42.13	$0.4290E44$
	2.0	4.197	30.01	$0.8579E44$
	$\delta_{cr} = 3.33$	13.5	13.5	$0.1430E45$
70	$\delta_e = 5.63E-26$	$0.899E-25$	66989	66989
	0.1	0.16	77.3	$0.4001E30$
	1.0	1.79	43.2	$0.4014E31$
	2.0	4.195	30.74	$0.8025E31$
	$\delta_{cr} = 3.352$	13.6	13.6	$0.1345E32$
40	$\delta_e = 1.94E-13$	$0.3099E-12$	21326	21326
	0.1	0.16	86.4	$0.3756E17$
	1.0	1.79	46.2	$0.3760E18$
	2.0	4.19	32.4	$0.7512E18$
	$\delta_{cr} = 3.395$	14.0	14.0	$0.1275E19$
20	$\delta_e = 2.275E-5$	$0.363E-4$	5005	5005
	0.1	0.16	119.6	$0.7750E8$
	1.0	1.79	55.1	$0.7708E9$
	2.0	4.18	37.3	$0.1549E10$
	$\delta_{cr} = 3.5033$	14.9	14.9	$0.271E10$
15	$\delta_e = 1.856E-3$	$0.296E-2$	2690	2690
	0.1	0.16	162.2	$0.5160E6$
	1.0	1.79	63.4	$0.5210E7$
	2.0	4.16	41.5	$0.1043E8$
	$\delta_{cr} = 3.5813$	15.6	15.6	$0.187E8$
8	$\delta_e = 0.5296$	0.895	632	632
	1.2	2.2	123.8	$0.421E4$
	2.2	4.7	64.2	$0.896E4$
	$\delta_{cr} = 3.902$	19	19	$0.1703E5$
4.5	$\delta_e = 4.509$	19.8	107	107
	4.62	22.63	64.04	162.9
	$\delta_{cr} = 4.767$	35.2	35.2	1986
$\tilde{\alpha} = 4.192$	$\delta_e = 5.034 = \delta_{cr}$	57	57	57

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TABLE 3

Values of $\tilde{K}_\infty$, v^* and $\bar{K}_\infty$ for some values of α and δ for the cylinder.

α	δ	$\tilde{K}_\infty$	v^*	$\bar{K}_\infty$
100	$\delta_e = 8.376E-39$	$0.124E-37$	105791	105791
	0.1	0.1503	41.06	$0.3148E43$
	1.0	1.838	19.80	$0.3148E44$
	$\delta_{cr} = 2.01$	7.71	7.71	$0.633E44$
70	$\delta_e = 4.365E-26$	$0.6445E-25$	51450	51450
	0.1	0.1503	42.56	$0.2946E30$
	1.0	1.837	20.25	$0.2946E31$
	$\delta_{cr} = 2.0194$	7.79	7.79	$0.595E31$
40	$\delta_e = 1.502E-13$	$0.2217E-12$	16457	16457
	0.1	0.1503	46.95	$0.2759E17$
	1.0	1.836	21.42	$0.2759E18$
	$\delta_{cr} = 2.045$	7.96	7.96	$0.564E18$
20	$\delta_e = 1.721E-5$	$0.254E-4$	3826	3826
	0.1	0.1503	62.23	$0.5767E8$
	1.0	1.833	24.8	$0.5767E9$
	$\delta_{cr} = 2.1092$	8.57	8.57	$0.1216E10$
15	$\delta_e = 1.367E-3$	$0.202E-2$	2021	2021
	0.1	0.1503	80.45	$0.3920E6$
	1.0	1.83	27.8	$0.3944E7$
	$\delta_{cr} = 2.1552$	8.9	8.9	$0.8506E7$
8	$\delta_e = 0.3578$	0.564	448	448
	0.8	1.39	65.8	$0.2260E4$
	1.6	3.53	29.5	$0.5290E4$
	$\delta_{cr} = 2.3456$	10.6	10.6	$0.811E4$
4.5	$\delta_e = 2.8077$	14	77.5	77.5
	$\delta_{cr} = 2.8625$	17.9	17.9	91
$\tilde{\alpha} = 4.002$	$\delta_e = 3.205 = \delta_{cr}$	33	33	33

3. Results for the slab, the sphere and the cylinder

For the slab, we have $0 \leq r \leq 1$, $\lambda_1 = \pi$ and $u_1(r) = \sqrt{2}\sin \pi r$. Results are presented in Table 1. We start with $\alpha = 100$, giving the values of δ_e and δ_{cr}. At

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$\delta = \delta_e$, v^* coincides with $\bar{K}_\infty$ and at $\delta = \delta_{cr}$, $\tilde{K}_\infty$ coincides with v^*. For $\delta_e < \delta < \delta_{cr}$, v^* is the threshold parameter. We decrease the value of α until we reach $\tilde{\alpha}$ at which δ_e and δ_{cr} coincide.

For the sphere, we have $0 \leqslant r \leqslant 1$, $\lambda_1 = \pi$, and $u_1(r) = \sin \pi r/(r\sqrt{2\pi})$. Results are presented in Table 2.

For the cylinder, we have $0 \leqslant r \leqslant 1$, $\lambda_1 = 2.405$ and $u_1(r) = J_0(\lambda_1 r)/J_1(\lambda_1)\sqrt{\pi}$. Results are presented in Table 3.

4. Concluding remarks

Using a method proposed by Kordylewski [2], Fenaughty *et al.* [1] recently obtained numerical critical values for the parameters δ and α for the three simple geometries. Their treatment is also numerical. Table 4 shows a comparison of the present result with theirs.

TABLE 4

Critical parameters as determined by the two methods

	Present result	Fenaughty *et al.*
Infinite slab (after adjusting for different scaling)	$\delta_{cr} = 5.227$ $\tilde{\alpha} = 4.069$	$\delta_{cr} = 5.2294$ $\tilde{\alpha} = 4.0687$
Infinite cylinder	$\delta_{cr} = 3.205$ $\tilde{\alpha} = 4.002$	$\delta_{cr} = 3.00617$ $\acute{\alpha} = 4.1304$
Sphere	$\delta_{cr} = 5.034$ $\tilde{\alpha} = 4.192$	$\delta_{cr} = 5.04081$ $\tilde{\alpha} = 4.1876$

Despite the slight discrepancy, it must be emphasized that the present integral equation approach produces not just $\tilde{\alpha}$ and δ_{cr}, but δ_e as well. For any given $\alpha > \tilde{\alpha}$, and $\delta_e < \delta < \delta_{cr}$, it also produces the number v^*, which is used to determine whether an arbitrarily given initial $\theta(r, 0)$ leads to the super-critical or sub-critical steady state.

Another observation that is perhaps worth making is that if one starts with the elliptic equation obtained from the governing equation by dropping the $\partial\theta/\partial t$ term and think of its multiple solutions as possible steady states, then since there may be more than two "steady state" solutions, it is difficult to attach the label

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"super-critical" or "sub-critical" to them. There is no such difficulty if one starts with the parabolic equation. Since the initial value problem has a unique solution, the steady state is either super-critical or sub-critical, depending on the initial data $\theta(r,0)$. The present work does in fact provide estimates on these two steady states, and the criterion on $\theta(r,0)$ that determines which one is reached.

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