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LINEARIZATION OF THE THERMAL EXPLOSION EQUATION AND THE STABILITY OF ITS SOLUTIONS FOR BOUNDARY CONDITIONS OF THE THIRD KIND

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A more rigorous derivation of the linearized equation of the thermal explosion previously obtained in [1] is given. By means of this equation the determination of the conditions for ignition of a reacting system involving conductive and convective heat transfer may be considerably simplified. The method of small perturbations is used to examine the stability of solutions of the steady-state equation of thermal explosion [2, 3] for boundary conditions of the third kind.

It is known [2, 3] that, within the limits of the steady-state approximation, thermal explosion theory leads, in the general case, to solution of the equation

$$\frac{\partial^2 \theta}{\partial x^2}+\frac{\partial^2 \theta}{\partial y^2}+\frac{\partial^2 \theta}{\partial z^2}+\delta \exp \theta=0 \tag{1}$$

with the condition

$$\left(\frac{\partial \theta}{\partial n}+\gamma \theta\right)\Big|_B=0. \tag{2}$$

Boundary problem (1), (2) ceases to have a real solution at some $\delta = \delta_*$ [2, 3, 5]. The value $\delta = \delta_*$ is the critical value, i.e., that at which ignition of the fuel mixture occurs. It is known [3, 5, 6] that when $\delta < \delta_*$ several solutions exist for boundary problem (1), (2), while at $\delta = \delta_*$ all the solutions merge, and the problem has a unique solution, i.e., the value $\delta = \delta_*$ is a branch point of the problem. Using the results of [7], it is easy to find the linear boundary problem

$$\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}+\delta \exp \theta_* v=0, \tag{3}$$

$$\left(\frac{\partial v}{\partial n}+\gamma v\right)\Big|_B=0, \tag{4}$$

whose eigenvalues coincide with the branch points of the nonlinear boundary problem (1), (2). In spite of the fact that Eq. (3) contains an unknown quantity $\theta_*(x,\ y,\ z,\ \delta_*)$, the linearized boundary problem (3), (4) considerably simplifies the determination of δ_* and may serve as a source of additional information. Thus, it was shown, with reference to many examples, in [6] that $\exp\theta_* = 2.71\ldots$* on the average, and δ_* may be determined with sufficient accuracy as the first eigenvalue of the boundary prlblem (3), (4) when $\theta_*(x,\ y,\ z,\ \delta_*) = 1$. In the two-dimensional case Eq. (3) coincides in form with the equation of vibration of a diaphragm [8], if we put

$$\exp[\theta_*(x,\ y,\ \delta_*)] = \rho(x,\ y)/F. \tag{5}$$

If θ_* has been determined, say, by experiment, δ_* may be determined using the diaphragm analogy, if one takes (5) into account and bears in mind that the boundary conditions correspond to an elastically supported diaphragm edge. Within the limits of the approximation $\theta_* = 1$ [1, 6, 9], the determination of δ_* using the diaphragm analogy is particularly simple. Upper and lower boundaries may also be determined, using the extermal properties of the eigenvalues of boundary problem (3), (4). Substituting $\theta_1 < \theta_*$, for example, into (3) instead of θ_*, we obtain, according to [10, 11], a value of δ_* that we know to be too high, and vice versa. The value of $\theta_1(x, y)$ is easily determined from Eq. (1), by replacing $\exp\theta$ with a value, equal to 1, known to be smaller, while $\theta_2 > \theta_*$ may be found from Eq. (1) by replacing $\exp\theta_*$ with the definitely larger value $\exp\theta_0$. Note that the method of successive approximations allow one to construct a sequence of upper and lower functions converging to θ_*, which we may then use to construct a sequence of upper and lower numbers converging to δ_*. According to [7], the determination of δ_* using an eigenvalue of boundary problem (3), (4) is necessary. The sufficiency of this determination for simple forms of reaction vessel (plane, cylindrical, and spherical) will be shown below.

*Note that the approximation $\exp\theta_* = e = 2.71\ldots$ was obtained in [9] from other consideration, but no consideration was given to the accuracy of the value of δ_* obtained.

Let us examine the unsteady equation of thermal conduction with distributed heat sources

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} + \frac{k}{x}\frac{\partial \theta}{\partial x} + \delta \exp \theta \tag{6}$$

and boundary conditions

$$\left.\frac{\partial \theta}{\partial x}\right|_{x=0} = 0, \quad \left.\left(\frac{\partial \theta}{\partial x} + \gamma\theta\right)\right|_{x=1} = 0. \tag{7}$$

We assume that the solution of boundary problem (6), (7) does not differ much from the solution of the corresponding steady-state boundary problem

$$\theta(x, t) = \theta_{st}(x) + u(x, t).$$

Substituting in the equation and discarding small quantities of second order and above, we obtain an equation for the perturbation u(x, t):

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{k}{x}\frac{\partial u}{\partial x} + \delta \exp \theta_{st}(x)\, u \tag{8}$$

with boundary conditions analogous to (7). We solve problem (8), (7) by separating the variables, putting $u = v(x) \cdot \exp(-\mu t)$ and substituting it in (8). We obtain an equation for v(x):

$$\frac{d^2 v}{dx^2} + \frac{k}{x}\frac{dv}{dx} + [\mu + \delta \exp \theta_{st}(x)]\, v = 0 \tag{9}$$

with boundary conditions analogous to (7). Thus, the problem of stability is reduced to that of determining the sign of the smallest eigenvalue of boundary problem (9), (7). If $\mu_0 > 0$, any initial temperature distribution is gradually dissipated. At $\mu_0 = 0$ this is no longer true, and at $\mu_0 < 0$ any initial temperature distribution steadily builds up, and an explosion occurs. Thus, $\mu_0 = 0$ is a limiting condition for ignition of the fuel mixture. We shall show that if $\theta_{st}(x)$ is the critical temperature profile in the steady-state theory of thermal explosion [2, 3], and δ is the critical value from the viewpoint of this theory, then $\mu_0 = 0$.

For a plane vessel the solution of boundary problem (1), (2) has the form

$$\theta_{st}(x) = \theta_0 - 2 \ln \operatorname{ch} sx. \tag{10}$$

A solution of (10) exists, if δ is determind from the expression

$$\delta = 2s^2(1 - \operatorname{th}^2 s) \exp\left(-\frac{2}{\gamma}\operatorname{th} s\right). \tag{10'}$$

At a certain critical value of $s = s_*$, δ has a maximum. The values s_* may be found from the equation

$$s_* \operatorname{th} s_* + s_*^2(1 - \operatorname{th}^2 s_*) + \gamma(s_* \operatorname{th} s_* - 1) = 0. \tag{10"}$$

This equation has a single positive root, which increases as γ increases. For a plane vessel when $\delta < \delta_*$ boundary problem (1), (2) has two solutions. At $s < s_*$ we obtain a first solution for which $\theta_0 < \theta_{0*}$, and at $s > s_*$ there is a second solution for which $\theta_0 > \theta_{0*}$. For a cylindrical vessel the solution of the steady-state problem (1), (2) has the form [12]:

$$\theta_{st}(x) = \theta_0 - 2 \ln(1 + mx^2). \tag{11}$$

A solution of (11) exists if

$$\delta = \frac{8m}{(1+m)^2} \exp\left[-\frac{4m}{\gamma(1+m)}\right]. \tag{11'}$$

The value $m = m_*$ corresponding to the maximum $\delta = \delta_*$ is given by

$$m_* = \frac{2}{\gamma}\left[\left(1 + \frac{\gamma^2}{4}\right)^{1/2} - 1\right]. \tag{12}$$

In this case the first and second solutions are similarly determined. For a spherical vessel the solution of problem (1), (2) may be written in the form [4]:

$$\theta_{st}(x) = \theta_0 - 2\int_0^{\xi}\left(x^{-2}\int_0^{x} y^2 \exp[\varphi(y)]\, dy\right) dx. \tag{13}$$

Making (13) satisfy boundary conditions (7), we obtain an equation

$$-\frac{2}{s}\int_0^s \xi^2 \exp[\varphi(\xi)]\, d\xi + \gamma\left[\theta_0 - 2\int_0^s\left(x^{-2}\int_0^x y^2 \exp[\varphi(y)]\, dy\right)\right] dx = 0 \tag{14}$$

for determining the values of δ for which a solution of the steady-state problem (1), (2) in a spherical vesses exists. Differentiating (14) with respect to θ_0 and using the condition $d\delta/d\theta_0 = 0$ [2, 3], we get an equation for the values $s = s_*$ corresponding to the extremum of δ:

$$s_*^{-1}(1-\gamma)\int_0^{s_*} x^2 \exp[\varphi(x)]\, dx + \gamma - s_*^2 \exp[\varphi(s_*)] = 0. \tag{15}$$

According to [5], by the change of variables $\psi = 2 + \xi\, d\varphi/d\xi$ and $p = \xi^2 \exp[\varphi(\xi)]$, Eq. (1) for a sphere may be reduced to the first-order equation

$$\frac{d\psi}{dp} = \frac{2(1-p)-\psi}{\psi p}.$$

It is easy to show that ξ always increases with variation of $\psi(p)$. Substituting ψ and p in (14), we have

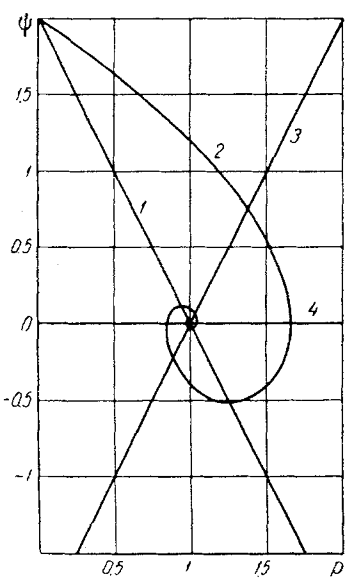
$$\delta = 2p \exp[(\psi - 2)/\gamma], \tag{16}$$

and instead of (15) we obtain

$$\psi_* = 2(p_* - 1)/(\gamma - 1). \tag{17}$$

Here the values ψ_* and p_* correspond to the values δ_* and s_*. They may easily be determined as the points of intersection of the curve $\psi(p)$ and the straight line given by (17). Having determined ψ_* and p_*, we may easily find δ_* from (16).

The figure shows a graph of $\psi(p)$ plotted up to the point (1.66, 0) using [13] and then finished qualitatively. The point (0, 2) is a singular point of the "node" type, while (1, 0) is one of the "focus" type [15]. It may be seen from the figure that there is an infinite number of points of intersection of the curve $\psi(p)$ with the above mentioned straight line. There are therefore infinitely many roots s_{i*} of (15).



Graphical solution of (17):
1) at $\gamma = 0$; 2) 1; 3) 2; 4) ∞.

It may also be seen from the figure that s_{i*} increases as γ increases. It is easy to show, using (14), that $d\theta/ds > 0$ at least for $\gamma \geq 1$, and that therefore the maximum temperature increases as s increases. We may also conclude from the figure that the curve $\delta(s)$ is not monotonic, but has an infinite number of alternating maxima and minima, diminishing in absolute value as s increases and tending asymptotically to the value $\delta = 2\exp(-2/\gamma)$ as $s \to \infty$. The extreme values of the curve $\delta(s)$ are given by (16) and (17). Substituting (10) into (9), for a plane reaction vessel we obtain

$$\frac{d^2v}{dx^2} + \left(\mu + \frac{2s^2}{ch^2 sx}\right)v = 0. \tag{18}$$

Similarly, substituting (11) into (9), for a cylindrical vessel we have

$$\frac{d^2v}{dx^2} + \frac{1}{x}\frac{dv}{dx} + \left[\mu + \frac{8m}{(1+mx^2)^2}\right]v = 0. \tag{19}$$

According to [4], the general solution of (18) at $\mu = 0$ is

$$v = C_1\, \mathrm{th}\, sx + C_2(1 - sx\, \mathrm{th}\, sx). \tag{20}$$

The general solution of (19) at $\mu = 0$ is

$$v = C_1\left[\frac{2 + (1 - mx^2)\ln x}{1 + mx^2}\right] + C_2\left(\frac{1 - mx^2}{1 + mx^2}\right). \tag{21}$$

Making (20) satisfy boundary conditions (7), we obtain an equation for determining the value s_* at which $\mu_0 = 0$. This equation coincides with (10"). Treating (21) similarly, we obtain an equation for determining the value m_* at which $\mu_0 = 0$. It is easy to find, by solving the equation, that this root coincides with (12). For a spherical vessel, according to [4], Eq. (9) has a solution at $\mu = 0$ satisfying the first of conditions (7):

$$v_1 = C_1(2 + \xi\, d\varphi/d\xi). \tag{22}$$

Substituting (22) into the second of conditions (7), we obtain (15). Thus, for three types of reaction vessel (plane, cylindrical, and spherical) we have shown that δ_* is an eigenvalue of the boundary problem (9), (7) at $\mu = 0$, since, determining values of $s_* m_*$ from (10"), (12), and (15) and substituting them in (10'), (11') and (14), we obtain $\delta = \delta_*$ for plane, cylindrical, and spherical vessels. For a spherical vessel, an infinite number of values δ_{i*} exist, and, according to the steady-state theory of thermal explosion [2, 3], the maximum of these should be chosen. At the same time, it has been shown that $\mu_0 = 0$ corresponds to the critical solution.

The function $f(s, x)$ in the neighborhood of $s = s_*$ may be represented in the form

$$f(s,\ x) = f(s_*,\ x) + 4s_* [1 - (s_* x)\,\mathrm{th}\,(s_* x)](1 - \mathrm{th}^2 s_* x)(s - s_*) + \ldots \tag{23}$$

Note that the sign of the second term in (23) depends on the difference in the square brackets. This is always positive and vanishes only at $x = 1$ if $s = s_*$ corresponds to $\gamma = \infty$. This is easy to establish from (10"). Thus, $f(s, x)$ increases as s increases. Then to $s_1 < s_*$, according to the first theorem on the properties of eigenvalues [11], there corresponds $\mu_0 > 0$, since $f(s_1, x) < f(s_*, x)$. For $s_2 > s_*$, we have $f(s_*, x) < f(s_2, x)$, and therefore $\mu_0 < 0$. Once having become negative, μ_0 cannot again become positive, since (10") has one positive root, and so $\mu_0 = 0$ uniquely.

In the neighborhood of $m = m_*$ the function $F(m, x)$ has the form

$$F(m,\ x) = F(m_*,\ x) + \frac{8(1 - m_* x^2)^2}{(1 + m_* x^2)^2}(m - m_*) + \ldots \tag{24}$$

Since, according to (12), for any γ m_* is always less than one, it follows from (24) that in the neighborhood of $m = m_*$ $F(m, x)$ is a monotonically increasing function of m. Then, by similar reasoning, we reach the conclusion that $\mu_0 > 0$ for $m_1 < m_*$, and hence the solution is stable, while that of (11) is unstable. Because there is an m_* for each γ, μ_0, having once become negative, will never be positive. Thus, solutions of the first type for plane and cylindrical vessels are always stable, and those of the second unstable. In the neighborhood of $s = s_*$ the function $\Phi(s, x)$ has the form

$$\Phi(s,\ x) = \Phi(s_*,\ x) + 2s_* \exp[\varphi(s_* x)]\,\psi(s_* x)(s - s_*) + \ldots \tag{25}$$

It is easy to see that the sign of the second term in (25) depends on the sign of $\psi(s_* x)$, which is positive for all x, if $s \leq s_{1*}$, and vanishes only at $x = 1$, if s_{1*} corresponds to $\gamma = \infty$. Then in the neighborhood of $s = s_{1*}$ $\Phi(s, x)$ is a monotonically increasing function, and, using the theorem cited [11], we may assert that, when $s < s_{1*}$, the solution of (13) satisfying this value of s is stable, while when $s > s_{1*}$ it is unstable. This method cannot be used to examine the stability of the solution in the neighborhood of all the other points $s = s_{1*}$, apart from the first, since in this case $\Psi(s_* x)$ may be negative for $x \sim 1$. Since the values of s at which $\mu_0 = 0$ are not unique, the method employed does not enable one to assert that the solution of (13) is unstable for all $s > s_{1*}$. The above investigation for a spherical reaction vessel is valid for the near neighborhood of $s = s_{1*}$, i.e., is local in character.

NOTATION

$\theta = E(T - T_0)/RT_0^2$ – dimensionless temperature; $\gamma = \alpha r/\lambda$ – Biot number; r – characteristic length of region D on which Eq. (1) is defined; B – boundary of region D; $\delta = \dfrac{qr^2 k_0 E \exp\left(-\dfrac{E}{RT_0}\right)}{RT_0^2}$; T_0 – ambient temperature; E – activation energy; q – calorific value of fuel; λ – thermal conductivity; k_0 – pre-exponential factor; R – universal gas constant; θ_0 – maximum dimensionless temperature in reaction vessel; θ_* – critical solution of boundary problem (1), (2) satisfying $\delta = \delta_*$; $\rho(x, y)$ – diaphragm density per unit surface area; F – diaphragm tension; $\theta_{st}(x)$ – solution of steady-state boundary problem (1), (2) for simple geometries; x, y, z – dimensionless coordinates; α – heat transfer coefficient; μ_0 – least eigenvalue of boundary problem (9), (7); $s = \sqrt{\delta \exp \theta_0/2}$, $\xi = sx$, $m = \dfrac{s^2}{4}$, C_1, C_2 – arbitrary constants; $t = \tau a/r^2$ – dimensionless time; a – thermal diffusivity; τ – time; $\varphi = \theta - \theta_0$; $f(s,\ x) = 2s^2(1 - \mathrm{th}^2 sx)$; $F(m,\ x) = \dfrac{8m}{(1 + mx^2)^2}$; $\Phi(s,\ x) = 2s^2 \exp[\varphi(sx)]$; k = 1, 2, 3 – for plane, cylindrical, and spherical vessels, respectively; $\delta_{i*} s_{i*}$ – successive roots of system of equations (14), (15); i = 1, 2, 3...; $\partial\theta/\partial n$ – derivative with respect to normal to boundary B.

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