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APPLICATION OF THE BIFURCATION THEORY TO EVALUATING CRITICAL CONDITIONS OF THE THERMAL EXPLOSION

1. Introduction. In recent years, much effort has been devoted to the mathematical study of problems of nonlinear heat generation. The most important of them, i.e. calculations of critical conditions of the thermal explosion, is a classical problem of the combustion theory.

The thermal explosion problem was formulated by Semenoff [20] who obtained the solution for a zero-dimensional model.

The thermal explosion theory, for bodies of one-dimensional geometry, started with the work of Frank-Kamenetsky who obtained analytically a critical parameter of the thermal explosion for an infinitely long layer [5]. The next analytical solution, for an infinitely long cylinder, was given by Chambre [4]. In the last two works the critical conditions of the thermal explosion were defined by a limit value of a certain parameter for which the heat generation equation was solvable.

Because of an essential difficulty in obtaining analytical solutions for more complicated shapes of bodies, approximate solutions have to be calculated. For example, Chambre [4] obtained the approximate solution for a sphere by means of tabulated functions.

In general, there are three distinct ways of solving this problem:

1. *By the expansion of the solution of the heat generation equation with infinite series* [3], [4]. In this method the coordinates of the point of the zero temperature gradient must be known, since the solution is expanded by series at this point.

2. *By the explicit integration of the heat generation equation and next by using tabulated functions* [21]. It seems that this method is limited to the cases of one-dimensional geometry.

3. *By the estimation of the critical parameters of the Laplace operator.* This method, first given probably by Hudjaev [6] and Joseph [7], does not make it possible to evaluate critical conditions of the thermal explosion in an exact way.

From the practical point of view, methods which allow to use the computer technique for calculating critical parameters are required. Examples of numerical calculations of critical parameters of the thermal explosion have been given by Parks [16] and by Anderson and Zienkiewicz [2]. In both works, critical parameters of the thermal explosion were defined as a limit value of some parameter of the heat generation equation for which numerical calculations become unstable.

This paper presents the method for evaluation of critical conditions of the thermal explosion and extinction based on the bifurcation theory.

In Section 2 the problem of the thermal explosion is formulated.

In Section 3 we collect (without proofs) some basic results about the nonlinear eigenvalue problem which occurs in the thermal explosion theory.

The necessary and sufficient conditions for the existence of bifurcation points of the heat generation equation are given in Section 4.

In Section 5 we present properties of solutions of the heat generation equation in a neighborhood of bifurcation points.

Section 6 contains two calculation procedures of critical parameters. Both procedures make it possible to calculate numerically the critical parameters by means of a computer.

Finally, in Section 7 we illustrate the presented method by some examples of numerical calculations of critical parameters of the thermal explosion.

2. Formulation of the problem. We consider a closed volume Ω with chemically reacting bodies inside. A result of the chemical reaction is heat generation at every point of this volume. Assuming that the efficiency $\dot{q}$ of heat sources per unit volume depends only on the temperature ϑ according to the Arrhenius law [23],

$$\dot{q} \sim \exp\left(-\frac{E}{R\vartheta}\right),$$

we obtain the model of the thermal explosion "without consumption" [5]. In this case there may exist stationary states of temperature distribution $\vartheta(x)$, which follow from the equality of the rate of heat generation and of loss of heat by the boundary surface $\partial\Omega$ (Fig. 1).

From the nonlinear dependence of the efficiency $\dot{q}$ of the heat source upon the temperature ϑ it follows that there may exist one of the two stationary states (Fig. 2). The first of them is characterized by low intensity of heat generation and by a body temperature almost equal to the temperature of assembly ϑ_0. The second state is characterized by a high rate of heat generation and a high maximum temperature of the body.

The transition from the one to the other state is discontinuous. Conditions under which an arbitrary small variation may cause a change of a stationary state are called *critical conditions of the thermal explosion (self-ignition) or extinction.*

The purpose of this paper is to give a method for the evaluation of critical conditions of the thermal explosion and extinction for arbitrary shapes of Ω.

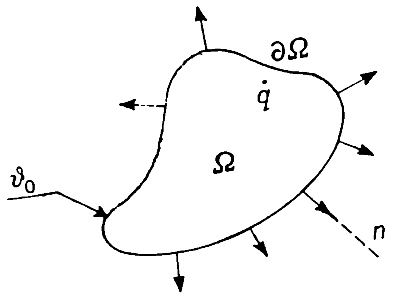

Fig. 1. A closed vessel with a chemically reacting mixture inside in the stationary state:

$$\int_{\Omega} \dot{q} d\Omega = \int_{\partial\Omega} q d(\partial\Omega),$$

$$q = -k\frac{\partial\vartheta}{\partial n}$$

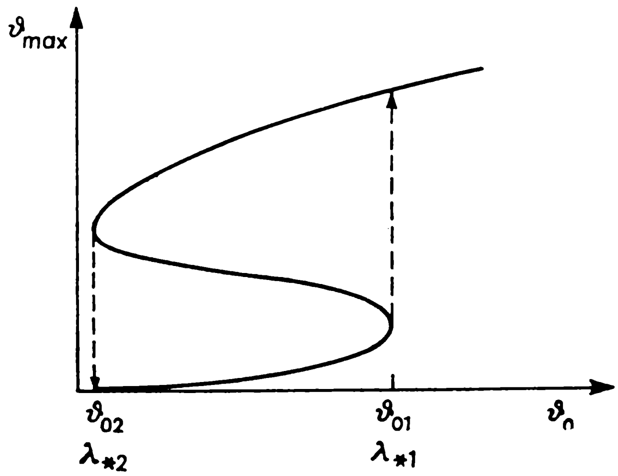

Fig. 2. Dependence of the maximum temperature of the body upon the temperature of the assembly for the sphere [16]

The mathematically formulated problem may be described as follows. Let Ω be a bounded domain in $\boldsymbol{R}^3$ with the smooth boundary $\partial\Omega$. The heat generation without reactant consumption is described by the nonlinear elliptic boundary value problem (NEBVP)

$$(1) \qquad Lu + \lambda f(u) = 0 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega,$$

where $L \equiv \nabla^2$ and u is a dimensionless temperature.

We assume a heat source f to be in the dimensionless form

$$f_2 = \exp\left(\frac{u}{1+\beta u}\right).$$

However, since for combustion the dimensionless parameter β is usually small, a simplified model of the thermal explosion with the approximate form of the heat source

$$f_1 = \exp(u)$$

will also be considered.

The dimensionless parameter λ plays an essential role in the formulation of critical conditions of the thermal explosion and extinction [5].

The basic assumption of this work is that the points of the thermal explosion and extinction are the points of bifurcation of the NEBVP (1). For this reason the linearized form of (1) will be considered:

$$L\varphi + \lambda f_u(u)\varphi = 0. \tag{2}$$

In the sequel, we shall denote by μ the principal eigenvalue of (2), and by φ the corresponding eigenvector.

3. Nonlinear eigenvalue problem (1). Denote by $\{\lambda\}$ a set of positive real values of λ for which there exist positive solutions of (1). The upper limit of $\{\lambda\}$, denoted by λ_c, is called a *critical value*. The following theorem shows how the nonlinear spectrum $\{\lambda\}$ depends upon the properties of the function f.

THEOREM 1 ([6], [9]). *Let $f(u) > 0$ for $u > 0$ and assume that the limit*

$$\lim_{u\to\infty} \frac{f(u)}{u}$$

exists (maybe, infinite). Then the NEBVP (1) *is solvable for every $\lambda > 0$ if and only if*

$$\lim_{u\to\infty} \frac{f(u)}{u} = 0.$$

Moreover, the critical value λ_c exists if and only if

$$\inf_{u>0} \frac{f(u)}{u} > 0.$$

From this theorem it follows that for $f = f_1$ the critical value λ_c exists and the nonlinear spectrum of (1) is of the form $(0, \lambda_c)$. In the case of $f = f_2$ the NEBVP (1) is solvable for every positive λ.

THEOREM 2 ([9]). *Assume that λ' belongs to the spectrum $\{\lambda\}$ of* (1). *Then the NEBVP* (1) *is solvable for every λ $(0 < \lambda < \lambda')$ and the solution u is an increasing function of λ for every $x \in \Omega$.*

In the case of the simplified heat source $f = f_1$ the properties of the implicit function $u(\lambda)$ are defined by the following

THEOREM 3 ([22]). *Suppose that $f(u) > 0, f_u(u) > 0$ and $f_{uu}(u) > 0$. Then a minimal solution of* (1) *depends continuously upon $\lambda \in (0, \lambda_c)$.*

In the case of the function $f = f_2$ the NEBVP (1) has a positive solution for any $\lambda > 0$, i.e. $\lambda_c = \infty$. Since the second derivative f_{uu} takes positive values for $u < 1/2\beta^2 - 1/\beta$ or negative values for $u > 1/2\beta^2 - 1/\beta$, the function f_2 may be convex or concave, respectively. Since we do not know a theorem similar to Theorem 3 for functions of this kind, we apply the inverse function theorem.

Let E_1 and E_2 be Banach spaces and let $Q = Q(u, \lambda)\colon E_1 \to E_2$ for λ and u such that $|\lambda - \lambda_0| \leqslant a$ ($\lambda \in \boldsymbol{R}$) and $\|u - u_0\| \leqslant b$ ($u \in E_1$). Suppose that $Q(u_0, \lambda_0) = 0$, i.e. u_0 is the solution of the equation

$$Q(u, \lambda) = 0 \tag{3}$$

for $\lambda = \lambda_0$.

We say that Q has a *Fréchet derivative* for $u \in E_1$ if there is a bounded linear operator $Q'\colon E_1 \to E_2$ such that

$$Q(u+h) - Qu = Q'h + \omega(u, h),$$

where

$$\lim_{\substack{h\to 0\\ h\in E_1}} \frac{\omega(u, h)}{\|h\|} = 0.$$

THEOREM 4 (the inverse function theorem [14]). *Assume that the operator Q for λ and u such that $|\lambda - \lambda_0| < a$ and $\|u - u_0\| < b$ satisfies the following conditions:*

1° *Q is continuous and $Q(u_0, \lambda_0) = 0$.*

2° *Q has the Fréchet derivative Q' which is continuous in the operator norm at the point (u_0, λ_0).*

3° *The linear operator $Q'(u_0, \lambda_0)$ is continuously invertible.*

Then there exist numbers $\alpha, \beta > 0$ such that for every λ with $|\lambda - \lambda_0| \leqslant \alpha$ equation (3) has a unique solution $u(\lambda)$ in the sphere $\|u - u_0\| \leqslant \beta$. The function $u(\lambda)$ is continuous.

In order to use Theorem 4 we transpose the NEBVP (1) into a fixed-point equation in a Banach space. By applying the Green function G for the operator L subject to the Dirichlet boundary conditions, NEBVP (1) is transposed into the following nonlinear integral equation of the Hammerstein type:

$$u(x) = \lambda \int_\Omega G(x, y) f[u(y)]\,dy, \qquad x \in \Omega. \tag{4}$$

Denoting by T the nonlinear operator

$$Tu = \int_\Omega G(\cdot, y) f[u(y)]\,dy,$$

we reduce the NEBVP (1) to the equation

$$u = \lambda T u \tag{5}$$

in which T is a completely continuous operator ([1]) of a certain Banach space ([2]) of functions on Ω [1]. It is clear that the operator

$$Q(u, \lambda) \equiv u - \lambda T u$$

is continuous.

The Fréchet derivative Q' exists and is of the form

$$Q' \equiv I - \lambda T',$$

where T',

$$T'v = \int_{\Omega} G(\cdot, y) f_u[u(y)] v(y)\, dy,$$

is a linear, completely continuous operator [13].

The operator Q' is *noninvertible* only if λ^{-1} is the eigenvalue of T'. In particular, for $f = f_2$ we infer that for every point of bifurcation λ_* (see below) there is at least one interval $[\lambda', \lambda_*) \subset \{\lambda\}$ for which $u(\lambda)$ is continuous.

4. Bifurcation points of (1). Consider a nonlinear operator equation (see [13])

$$\psi = F(\psi, \lambda), \quad F(0, \lambda) = 0. \tag{6}$$

The real number λ_* is called a *point of bifurcation of the operator* F if for every $\varepsilon > 0$ there exists a number λ which satisfies the inequality $|\lambda - \lambda_*| < \varepsilon$ and for which equation (6) has at least one nontrivial solution yielding $|\psi(\lambda)| < \varepsilon$.

Assume that $F(x, \lambda)$ has at $x = 0$ the Fréchet derivative F'. Then the inverse function theorem implies the necessary condition for the existence of a bifurcation point.

THEOREM 5 ([13]). *If* $[F'(0, \lambda_*) - I]$ *is a continuous invertible operator, then* λ_* *cannot be a point of bifurcation.*

We are interested in operators for which the Fréchet derivative takes the form

$$F'(0, \lambda) \equiv \lambda B, \tag{7}$$

([1]) T is called *completely continuous* if T is continuous and maps a closed bounded subset into a compact set [11].

([2]) In the sequel, we assume that $E_1 = E_2 = C_0(\Omega)$, where $C_0(\Omega)$ denotes the set $\{v \in C(\Omega): v = 0 \text{ on } \partial\Omega\}$.

where B is a linear continuous operator. Then from Theorem 5 it follows that the necessary condition for λ_* to be a point of bifurcation of (6) is that λ_*^{-1} belongs to the spectrum of B.

A sufficient condition for the existence of a bifurcation point of (6) follows from the analysis of the vector field (see [15])

$$\Phi_\lambda \psi \equiv \psi - F(\psi, \lambda). \tag{8}$$

According to the assumed form of the operator F, the index of (6) is defined by $i(F) = (-1)^m$, where m is the multiplicity of an eigenvalue of B.

THEOREM 6 ([15]). *If λ_*^{-1} is an eigenvalue of B of odd multiplicity, then λ_* is a bifurcation point of* (6).

Now we return to the fixed point of equation (5). Since the operator T does not have the property $T(0) = 0$, we introduce an operator

$$A(\psi, \lambda) = \lambda T[u(\lambda)+\psi] - u(\lambda),$$

where $\lambda \in \{\lambda\}$ and $u(\lambda)$ is a solution of (1). The operator A is also completely continuous and $A(0, \lambda) = 0$, $A' = \lambda T$. In such a way we replace (5) by

$$\psi = A(\psi, \lambda). \tag{9}$$

THEOREM 7 ([1], [13]). *The eigenvalue problem*

$$T'\varphi = \lambda^{-1}\varphi$$

has the largest eigenvalue λ_*^{-1} which is positive and simple. There exists exactly one normalized eigenvector φ corresponding to the eigenvalue λ_*^{-1}, and it can be chosen to be positive.

It is an immediate consequence of Theorems 5-7 that if λ_*^{-1} is the largest eigenvalue of T', then λ_* is the bifurcation point of (9), and hence of (5). From the equivalence of the fixed-point equation (5) and NEBVP (1) it follows that if λ_* is the principal eigenvalue of (2), then λ_* is the bifurcation point of (1).

5. Properties of the bifurcation solutions of (1). In order to obtain the properties of solutions of the NEBVP (1) in a neighborhood of the bifurcation point λ_*, we expand the left-hand side of equation (1) in the Taylor series at the point (λ_*, u_*) and obtain

$$L\psi + \lambda f_u(u_*)\psi + \lambda[\tfrac{1}{2}f_{uu}(u_*)\psi^2 + O(\psi^3)] = -\varepsilon f(u_*), \tag{10}$$

where $\psi = u - u_*$ and $\varepsilon = \lambda - \lambda_*$. Let us put

$$S(\lambda)\psi = L\psi + \lambda f_u(u_*)\psi, \quad C\psi \equiv \tfrac{1}{2}f_{uu}(u_*)\psi^2, \quad D\psi \equiv O(\psi^3), \tag{11}$$

where C is the homogeneous operator of second order with the properties

$$\|Cv_1 - Cv_2\| \leqslant q_0 r \|v_1 - v_2\| \qquad (\|v_1\|, \|v_2\| \leqslant r), \tag{12}$$

r being a positive constant, and D is the operator of order higher than two and such that

$$\|Dv_1 - Dv_2\| \leqslant q_1(r) \|v_1 - v_2\| \qquad (\|v_1\|, \|v_2\| \leqslant r), \tag{13}$$

where $q_1(r) = o(r)$.

Substituting (11) into (10) we get

$$S(\lambda)\psi + \lambda(C+D)\psi = -\varepsilon f(u_*). \tag{14}$$

Denote by $N(S)$ the zero space of the operator $S(\lambda_*)$. The space $N(S)$ is one-dimensional with a positive eigenvector φ as a base vector.

Further we denote by P_0 a linear operator which projects $C_0(\Omega)$ into $N(S)$ and is defined by

$$P_0 v = \eta(v)\varphi, \qquad v \in C_0(\Omega), \tag{15}$$

where $\eta(v)$ is the scalar product

$$\langle v, \varphi \rangle = \int_\Omega v(x)\varphi(x)\,dx$$

and $\eta\big(f_u(u_*)\varphi\big) = 1$.

The linear operator $P^0 = I - P_0$ projects $C_0(\Omega)$ into an invariant subspace $C_{0i}(\Omega)$ for $S(\lambda_*)$. In this way every element $v \in C_0(\Omega)$ has the decomposition

$$v = P^0 v + \eta(v)\varphi. \tag{16}$$

Assume a solution of (14) is of the form

$$\psi = P^0\psi + a\varphi, \tag{17}$$

where $a = \eta(\psi)$.

We show that a determines uniquely the qualitative dependence of the solution ψ on a parameter ε. Applying the functional η in (14) we obtain the scalar equation

$$\varepsilon a + \lambda\eta(C\psi + D\psi) = -\varepsilon\eta[f(u_*)], \tag{18}$$

and hence

$$\varepsilon = -\frac{\eta(C\psi) + \eta(D\psi)}{a + \eta[f(u_*)]}. \tag{19}$$

Projecting now equation (14) into $N(S)$ we obtain

$$S(\lambda)P^0\psi + \lambda P^0(C\psi + D\psi) = -\varepsilon P^0 f(u_*). \tag{20}$$

Since $C_{0i}(\Omega)$ is invariant for $S(\lambda_*)$, there exists an inverse operator $R(\lambda) = S(\lambda)^{-1}$ for values λ which differ sufficiently small from the value λ_* [13]. Hence equation (20) takes the form

$$P^0\psi = -\lambda R(\lambda)P^0(C\psi + D\psi) - \varepsilon R(\lambda)P^0 f(u_*).$$

By (19) we have

$$P^0\psi = -\lambda R(\lambda)P^0\left\{C\psi + D\psi - \frac{\eta(C\psi)+\eta(D\psi)}{a+\eta[f(u_*)]}f(u_*)\right\},$$

whence, using (17), we obtain the following equation which permits to estimate $P^0\psi$ as a function of a:

$$P^0\psi = \lambda R(\lambda)P^0Q(a)(P^0\psi), \tag{21}$$

where

$$Q(a)(P^0\psi) = -C(P^0\psi + a\varphi) - D(P^0\psi + a\varphi) + \\ + \frac{\eta[C(P^0\psi + a\varphi)] + \eta[D(P^0\psi + a\varphi)]}{a+\eta[f(u_*)]}f(u_*).$$

It follows from properties (12) and (13) of the operators C and D that the operator $Q(a)$ satisfies the Lipschitz conditions [13], i.e.

$$\|Q(a)v_1 - Q(a)v_2\| \leqslant q_3\|v_1 - v_2\|,$$

where the constant q_3 depends upon a real $r > 0$ ($\|v_1\|, \|v_2\| \leqslant r$) and may be arbitrarily small because

$$\lim_{r\to 0} q_3(r) = 0.$$

Since $R(\lambda)P^0$ has a bounded norm on $C_{0i}(\Omega)$, we may choose a sufficiently small r_0 ($r_0 > r > 0$) such that, for a with $|a| < r$, the operator $R(\lambda)P^0Q(a)$ in the sphere $M = \{\|v\| \leqslant r : v \in C_{0i}(\Omega)\}$ is a contraction. Consequently, equation (21) has exactly one solution $P^0\psi$ in the sphere M for every a with $|a| \leqslant r$, $r \leqslant r_0$.

Next, from (21) (with $R = R(\lambda)$) we get

$$\|RP^0Q(a)0\| \leqslant \|R\|\,\|P^0\|\left\{\|C(a\varphi) + D(a\varphi)\|\left[1 + \frac{\|\eta\|\,\|f(u_*)\|}{a+\eta[f(u_*)]}\right]\right\}$$

and, further, by (12), (13) and by the inequalities

$$\frac{1}{a+\eta[f(u_*)]} \leqslant \frac{1}{\eta[f(u_*)] - |a|} \leqslant \left(1 + 2\frac{|a|}{\eta[f(u_*)]}\right)\frac{1}{\eta[f(u_*)]} \quad \text{for } |a| < \frac{1}{2},$$

we obtain the estimate

$$\|R(\lambda)P^0Q(a)0\| \leqslant q_4|a|^2, \quad q_4 = O(1). \tag{22}$$

From (22) and (21) we get

$$\begin{aligned}\|P^0\psi\| &= \lambda\|RP^0Q(a)(P^0\psi)\| \\ &\leqslant \lambda[\|RP^0Q(a)0\| + \|RP^0Q(a)(P^0\psi) - RP^0Q(a)0\|] \\ &\leqslant \lambda[q_4|a|^2 + q_3\|R\|\,\|P^0\|\,\|P^0\psi\|],\end{aligned}$$

whence

$$\|P^0\psi\| \leqslant \frac{q_4|a|^2}{1-\lambda q_3\|R\|\,\|P^0\|} \leqslant q_5|a|^2, \qquad R = R(\lambda). \tag{23}$$

Introducing the scalar function

$$\xi(a) = \eta[C(P^0\psi + a\varphi)] - \eta[C(a\varphi)] + \eta[D(P^0\psi + a\varphi)],$$

we obtain equation (19) in the form

$$\varepsilon = \lambda\frac{\eta C(a\varphi) + \xi(a)}{a + \eta[f(u_*)]}.$$

By the properties of the operator C and then by (23) we get

$$\begin{aligned}\|\eta[C(P^0\psi + a\varphi)] - \eta[C(a\varphi)]\| &\leqslant k\|\eta\|[\|P^0\psi\| + 2|a|]\|P^0\psi\| \\ &\leqslant k\|\eta\|[q_5|a|^2 + 2|a|]q_5|a|^2 \leqslant q_6(a)|a|^2, \qquad |a| \leqslant r,\end{aligned} \tag{24}$$

where k is a positive constant. Since the operator D contains terms of third order and higher, we have

$$\|Dv\| \leqslant q_7\|v\|^3, \qquad q_7 = O(1),$$

and hence

$$\begin{aligned}\|\eta[D(P^0\psi + a\varphi)]\| &\leqslant \|\eta\|q_7\|P^0\psi + a\varphi\|^3 \\ &\leqslant \|\eta\|q_7(|a| + q_5|a|^2)^3 \leqslant q_8(a)|a|^2.\end{aligned} \tag{25}$$

For sufficiently small r_0 ($|a| < r < r_0$) it follows from (24) and (25) that

$$\|\xi(a)\| \leqslant a^2[q_6(a) + q_8(a)],$$

where

$$\lim_{|a|\to 0} q_6(a) = \lim_{|a|\to 0} q_8(a) = 0.$$

Suppose that $\eta(C\varphi) \neq 0$. Then the function $\xi(a)$ takes the form (see [10], [13], [14])

$$\xi(a) = a^2\eta(C\varphi)\nu(a).$$

Clearly,

$$\lim_{|a|\to 0} \nu(a) = 0.$$

Finally, equation (19) can be written as

$$\varepsilon = -\lambda a^2 \eta(C\varphi)\frac{1+\nu(a)}{\eta[f(u_*)]+a}. \tag{26}$$

Hence for sufficiently small r_0 we have

$$\operatorname{sign}\varepsilon = -\operatorname{sign}\eta(C\varphi). \tag{27}$$

From (26) it follows that equation (14) has nontrivial solutions with a small norm if $|\varepsilon| \neq 0$. There are no solutions if ε does not satisfy (27). For ε fulfilling equality (27) there are two solutions ($a_1 > 0$ and $a_2 < 0$) which converge to zero as $\varepsilon \to 0$.

The geometric form of the results obtained is shown in Fig. 3. From the point of view of physics it means that for $f = f_1$ there is one point of bifurcation of the type as shown in Fig. 3a. This point corresponds to the point of thermal explosion for the simplified model. In the case of $f = f_2$, two bifurcation points of the type as in Figs. 3a and 3b can occur, since $\eta(C\varphi)$ can take positive and negative values. One of these bifurcation points corresponds to the thermal explosion λ_{*1} and the other one to the extinction λ_{*2} (Fig. 2).

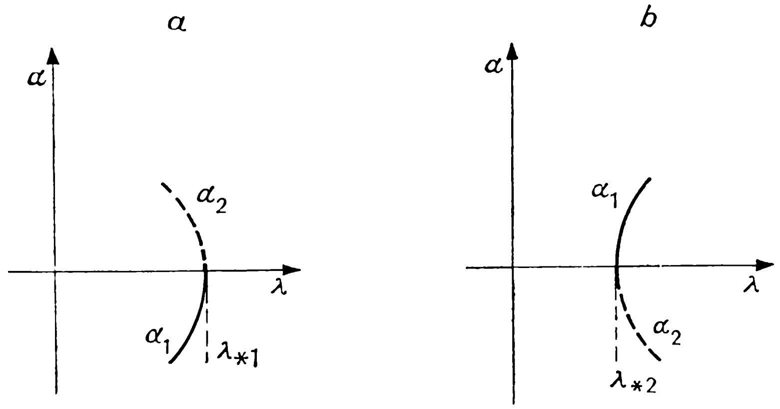

Fig. 3. Geometric form of small solutions in a neighborhood of the bifurcation points
a – for $\eta(C\varphi)>0$, b – for $\eta(C\varphi)<0$, ——— stable solution, ----- unstable solution

6. Calculation procedures of critical parameters. For the calculation of singular points of the NEBVP (1) a nonstationary calculation procedure will be suggested. We consider the following system of equations:

$$\frac{du}{dt} = Lu+\lambda f(u), \tag{28}$$

$$\frac{d\varphi}{dt} = L\varphi+\lambda f_u(u)\varphi, \tag{29}$$

$$\frac{d\lambda}{dt} = \mu(\lambda)-\lambda. \tag{30}$$

The desired solutions u, φ, λ of (1), (2) will be the limits (for $t \to \infty$) of solutions of (28)-(30). We have chosen (30), since $d\lambda/dt \to 0$ as $t \to \infty$ implies $\lambda = \mu$, which is a necessary and sufficient condition for λ to be the bifurcation point of (1). We show that (30) in the limit takes the form $\lambda = \mu$.

Assume that λ is a function of t such that

$$\frac{d\lambda}{dt} = \mu[\lambda(t)] - \lambda(t). \tag{31}$$

Multiplying equation (31) by $d\mu(\lambda)/d\lambda - 1$ we obtain

$$\frac{d\ln(\mu-\lambda)}{dt} = \frac{d\mu}{d\lambda} - 1. \tag{32}$$

First we determine the derivative $d\mu/d\lambda$ in the neighborhood of the bifurcation point of equation (1).

If $\lambda_1 < \lambda_2 < \lambda_*$, then two corresponding solutions u_1, u_2 of (1) exist. Assume that u_1, u_2 are minimal solutions of (1). Let μ_1, φ_1 and μ_2, φ_2 be principal eigenvalues and eigenvectors of (2) corresponding to values λ_1 and λ_2. Then the following equation holds:

$$L\varphi_1 + \mu_2 f_u(u_2)\varphi_1 = \mu_2 f_u(u_2)\varphi_1 - \mu_1 f_u(u_1)\varphi_1. \tag{33}$$

The right-hand side of (33) must be orthogonal to φ_2, so

$$\langle \mu_2 f_u(u_2)\varphi_1 - \mu_1 f_u(u_1)\varphi_1, \varphi_2 \rangle = 0. \tag{34}$$

Using the mean value theorem for $f_u(u_2)$ we can write (34) in the form

$$(\mu_2 - \mu_1)\langle f_u(u_1)\varphi_1, \varphi_2\rangle = -\mu_2 \langle f_{uu}[u_1 + \theta(u_2 - u_1)](u_2 - u_1)\varphi_1, \varphi_2\rangle, \quad 0 \leqslant \theta \leqslant 1. \tag{35}$$

If we put $u_i - u_* \cong a_i\varphi_*$, where φ_* is the eigenfunction corresponding to λ_*, we can write approximately

$$u_2 - u_1 \cong (a_2 - a_1)\varphi_*.$$

Then equation (35) becomes

$$(\mu_2 - \mu_1)\langle f_u(u_1)\varphi_1, \varphi_2\rangle = -(a_2 - a_1)\mu_2 \langle f_{uu}[u_1 + \theta(u_2 - u_1)]\varphi_*\varphi_1, \varphi_2\rangle. \tag{36}$$

Since the principal eigenvalue μ is simple, in the limit for $|\lambda_2 - \lambda_1| \to 0$ we have

$$|\mu_2 - \mu_1| \to 0, \qquad \|\varphi_2 - \varphi_1\| \to 0,$$

and if $\lambda_1, \lambda_2 \to \lambda_*$, then $\varphi_1, \varphi_2 \to \varphi_*$. Dividing (36) by $\lambda_2 - \lambda_1$, in the limit for $|\lambda_2 - \lambda_1| \to 0$ we have

$$\frac{d\mu}{d\lambda} = -\mu \frac{da}{d\lambda} \langle f_{uu}(u)\varphi^2, \varphi_*\rangle, \tag{37}$$

where φ corresponds to μ and is normalized by $\langle f_u\varphi, \varphi\rangle = 1$.

At the bifurcation point of the type as shown in Fig. 3a we have $\langle f_{uu}\varphi_*^2, \varphi_*\rangle > 0$, and so in a sufficiently small neighborhood of λ_* we get $\langle f_{uu}\varphi^2, \varphi_*\rangle > 0$. From the inverse function theorem it results [14] that the function $u(\lambda)$, as a solution of equation (1), has a derivative $du/d\lambda$ which is nonnegative (Theorem 2), and hence $da/d\lambda \geqslant 0$.

Equation (37) indicates $d\mu/d\lambda \leqslant 0$ and, finally, equation (32) implies the estimate

$$|\mu - \lambda| \leqslant M \exp\left[\int_0^t \left(\frac{d\mu}{d\lambda} - 1\right) ds\right] \leqslant M \exp[-t], \tag{38}$$

where M is a positive constant.

For convenience of computations we replace (30) by

$$\frac{d\lambda}{dt} = C_1 \langle L\varphi + \lambda f_u \varphi, g\rangle, \tag{30'}$$

where C_1 is a positive constant. We have chosen (30′), since the equation

$$L\varphi + \mu f_u(u)\varphi = 0$$

implies

$$\mu = -\frac{\langle L\varphi, g\rangle}{\langle f_u\varphi, g\rangle} \tag{39}$$

for every $g(x)$ such that $\langle f_u(u)\varphi, g\rangle \neq 0$. We now substitute (39) with $\varphi(t, x)$ instead of φ into (30) and get

$$\frac{d\lambda}{dt} = -\frac{\langle L\varphi + \lambda f_u\varphi, g\rangle}{\langle f_u\varphi, g\rangle}.$$

In the sequel we replace $\langle -f_u\varphi, g\rangle$ by a positive constant C_1^{-1}.

Equation (30′) was used in [18] for solving the linear eigenvalue problem of type (2). It was proved that for an arbitrary negative function $g(x)$ the solutions of (29) and (30′) converge to the principal eigenvalue μ and to the corresponding eigenfunction φ.

In the case of the second bifurcation point, where $\langle f_{uu}\varphi_*^2, \varphi_*\rangle < 0$, it follows from (37) that $d\mu/d\lambda \geqslant 0$ for the stable solution $a_1 > 0$ (Fig. 3). Attempts to calculate coordinates of this bifurcation point by procedure (28)-(30′) failed.

Another calculating procedure, based on the suggestion of Keller and Langford [10], is proposed:

$$\frac{du}{dt} = Lu + \lambda f(u), \tag{40}$$

$$\frac{d\varphi}{dt} = L\varphi + \mu f_u(u)\varphi, \tag{41}$$

$$\frac{d\mu}{dt} = C_1 \langle L\varphi + \mu f_u(u)\varphi, g\rangle, \tag{42}$$

$$\frac{d\lambda}{dt} = -C_2 \left\langle C_3 \frac{du}{dt} - u f_u(u) + f(u), \varphi \right\rangle. \tag{43}$$

We have no proof of the convergence of this procedure, but we comment on the choice of constants C_2 and C_3. Since the solutions of (41) and (42) converge expotentially to the principal eigenvalue and to the eigenvector of (2) [18], we omit these equations in the simplified analysis of the linearized stability of the system of equations (40)-(43). Assume that $\lambda > \lambda_{*2}$. Then equations (40)-(43) may take the approximate forms

$$\frac{da}{dt} = \varepsilon \langle f, \varphi\rangle,$$

$$\frac{d\varepsilon}{dt} = -\varepsilon C_2 C_3 \langle f, \varphi\rangle - a C_2 \langle u f_{uu}\varphi, \varphi\rangle,$$

where $\varphi = \varphi_*$, $u - u_* \cong a\varphi$, $\varepsilon = \lambda - \lambda_*$, $f = f(u_*)$, $f_{uu} = f_{uu}(u_*)$. The roots of the equation

$$\det(A - sI) = 0,$$

where

$$A = \begin{vmatrix} 0 & \langle f, \varphi\rangle \\ -C_2 \langle u f_{uu}\varphi, \varphi\rangle & -C_2 C_3 \langle f, \varphi\rangle \end{vmatrix},$$

are of the form

$$s_{1,2} = -\frac{1}{2} C_2 C_3 \langle f, \varphi\rangle \left[1 \pm \sqrt{1 + \frac{4\langle u f_{uu}\varphi, \varphi\rangle}{C_2 C_3^2 \langle f, \varphi\rangle^2}}\right].$$

Clearly, the system of equations (40)-(43) may be stable only if $\langle u f_{uu}\varphi, \varphi\rangle / C_2 < 0$.

The constants C_2 and C_3 may be chosen in such a way that the solutions $a(t)$ and $\varepsilon(t)$ are periodic or aperiodic. It was shown in [12] that, in the case of the slab and the sphere, oscillations appeared when $1/C_2 C_3^2 > 100$.

7. Results of calculations. Equations (28)-(30′) and (40)-(43) were solved numerically [12] by the finite-difference technique using the explicit and implicit methods [17].

The convergence of procedure (28)-(30′) illustrates the dependence of the parameter λ_* and the maximum temperature u_* on the grid density $h = 2a/N$ for the slab and the simplified heat source f_1 (Table 1). An in-

TABLE 1. Dependence of the parameter λ_* and the maximum temperature u_* on the grid density for the slab

h	λ_*	u_*
$2a/10$	0.87388	1.18348
$2a/20$	0.87733	1.18598
$2a/40$	0.87831	1.18644

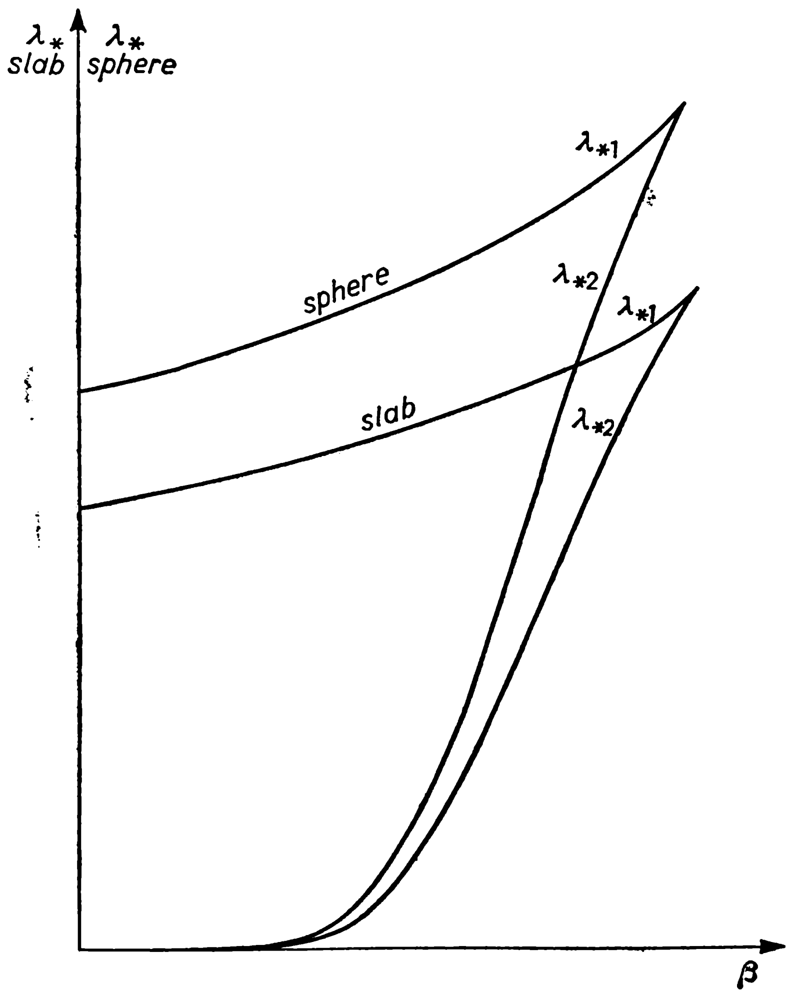

Fig. 4. Dependence of critical parameters λ_* of thermal explosion and extinction for the slab and the sphere on the parameter β [12]

crease of the grid density causes the convergence of results of the numerical calculations to the analytical solution [5]. The results obtained by procedure (28)-(30′) for other simple shapes were in good agreement with those given in the literature [12].

In the case of the limited heat source f_2 both procedures were used, the first for calculations of thermal explosion points and the second for calculations of extinction points. In Fig. 4 the dependence of the critical parameters λ_{*1}, λ_{*2} on the parameter β for the slab and for the sphere is presented.

Experience [12] showed that procedure (28)-(30′) is characterized by good stability and small sensitivity on the selection of initial conditions. Procedure (40)-(43) is slowly convergent and its stability depends on the choice of initial conditions, particularly for small values of the parameter β.

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ZASTOSOWANIE TEORII BIFURKACJI DO WYZNACZANIA WARUNKÓW KRYTYCZNYCH EKSPLOZJI TERMICZNEJ

STRESZCZENIE

W pracy wyznacza się punkty bifurkacji nieliniowego równania eliptycznego

$$Lu + \lambda f(u) = 0,$$

opisującego przewodnictwo i generację ciepła w procesie spalania. Współrzędne tych punktów określają warunki samozapłonu i gaśnięcia.

Wykazano, że dla wartości parametru λ, równej pierwszej wartości własnej zlinearyzowanego równania

$$L\varphi + \lambda f_u(u)\varphi = 0,$$

następuje bifurkacja rozwiązania.

Analizowano warunki zbieżności dwóch procedur obliczeniowych, przeznaczonych do wyznaczania punktów samozapłonu i gaśnięcia. W przypadku punktu samozapłonu wykazano zbieżność procedury obliczeniowej dla warunków początkowych dostatecznie bliskich punktowi bifurkacji.