

ASYMPTOTIC ANALYSIS OF CRITICAL CONDITIONS OF SELF-IGNITION FOR DISTRIBUTED MODELS

Gorelov G. N.

Samara State Aerospace University

Russia, 443013, Samara, box 9525

e-mail: georg@sgpp.ru

Abstract

The paper is devoted to the thermal explosion problem in the case of autocatalytic reaction given both heat transfer and diffusion. By means of the method of integral manifolds there are investigated critical regimes and are found critical values of parameter for plane-parallel and for cylindrical reactors.

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1 Introduction

The problem of evaluation of critical regimes thought of as regimes separating the regions of explosive and nonexplosive ways of chemical reactions is the main mathematical problem of the thermal explosion theory.

Investigation of critical phenomena of the thermal explosion theory was hold by N. N. Semenov [1], Ya. B. Zeldovich [2], D. A. Frank-Kamenetsky [3], O. M. Todes and P. V. Melent'ev [4], A. G. Merzhanov and F. I. Dubovitsky [5], B. Grey [6] et al. Because of considerable difference between velocities of thermal and concentrational changes, singularly perturbed systems of differential equations serve as mathematical models of such problems. But in the above works the authors restrict their consideration to the study of zero order approximation. It does not let them explain the strong parametric sensitivity of this problem as well as to examine the transformation of solutions in the vicinity of the limit of selfignition.

In the works [7, 8, 9] it was proposed to use the stable-unstable integral manifold as a mathematical model of the critical regime of the autocatalytic reaction within investigation of the lumped model. This approach permits to work out the algorithms of asymptotic representations of the critical values of the parameter of initial conditions and to describe the transfer regimes. The lumped model is investigated in details in the report of V. A. Sobolev at present conference.

Such approach appeared to be fruitful in the case of distributed model in the problem of thermal explosion.

2 The Main Problem

Consider nonlinear singularly perturbed parabolic system

$$\varepsilon \frac{\partial \theta}{\partial \tau} = \frac{1}{\delta} \left(\frac{\partial^2 \theta}{\partial \xi^2} + \frac{n}{\xi} \frac{\partial \theta}{\partial \xi} \right) + \varphi(\eta) \exp \left(\frac{\theta}{1 + \beta \theta} \right), \quad (1)$$

$$\varepsilon \frac{\partial \eta}{\partial \tau} = \frac{1}{\rho} \left(\frac{\partial^2 \eta}{\partial \xi^2} + \frac{n}{\xi} \frac{\partial \eta}{\partial \xi} \right) + \varepsilon \varphi(\eta) \exp \left(\frac{\theta}{1 + \beta \theta} \right) \quad (2)$$

with boundary conditions

$$\left. \frac{\partial \theta}{\partial \xi} \right|_{\xi=0} = 0, \quad \theta \Big|_{\xi=1} = 0, \quad \left. \frac{\partial \eta}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \frac{\partial \eta}{\partial \xi} \right|_{\xi=1} = 0 \quad (3)$$

and initial conditions

$$\theta \Big|_{\tau=0} = 0, \quad \eta \Big|_{\tau=0} = 0. \quad (4)$$

This is a mathematical model of the problem of thermal explosion given heat transfer and diffusion in the case of autocatalytic combustion process. Here θ is a dimensionless temperature, η is a dimensionless rate of combustion, τ is a dimensionless time, ε and β are small positive parameters, δ is a Frank-Kamenetsky criterion, that is the scalar parameter, characterizing initial state of the system. Depending on its value, reaction either is explosive or proceeds slowly. The value of parameter δ separating slow and explosive regimes is called critical. Function $\varphi(\eta)$ determines the law according to which the reaction proceeds: for $\varphi(\eta) = \eta$ we have the first order reaction, for $\varphi(\eta) = \eta^n$ it is the n -th order reaction, and for $\varphi(\eta) = \eta(1 - \eta)$ it is an autocatalytic one.

Using the method of integral manifolds, the critical value of δ is calculated as an asymptotic series with respect to degrees of the small parameter ε

$$\delta = \delta_0(1 + \delta_1\varepsilon) + O(\varepsilon^2), \quad (5)$$

where critical regimes are modelled by the duck-trajectories. For $n = 0$ (plane-parallel reactor) $n = 1$ (cylindrical reactor) corresponding values of δ_0 and δ_1 are estimated.

3 Critical conditions of the plane-parallel reactor

Setting $n = 0$ in (1)–(2), in the case of plane-parallel reactor we obtain the system

$$\begin{aligned} \varepsilon \frac{\partial \theta}{\partial \tau} &= \eta(1 - \eta)e^\theta + \frac{1}{\delta} \frac{\partial^2 \theta}{\partial \xi^2}, \\ \varepsilon \frac{\partial \eta}{\partial \tau} &= \varepsilon \eta(1 - \eta)e^\theta + \frac{1}{\varrho} \frac{\partial^2 \eta}{\partial \xi^2}, \end{aligned} \quad (6)$$

with boundary conditions

$$\left. \frac{\partial \theta}{\partial \xi} \right|_{\xi=0} = 0, \quad \theta \Big|_{\xi=1} = 0; \quad \left. \frac{\partial \eta}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \frac{\partial \eta}{\partial \xi} \right|_{\xi=1} = 0. \quad (7)$$

One-dimensional slow integral manifold corresponds to the critical regime. This manifold can be found in a parametric form

$$\begin{aligned} \theta &= \theta(v, \xi, \varepsilon) = \theta_0(v, \xi) + \varepsilon \theta_1(v, \xi) + O(\varepsilon^2), \\ \eta &= \eta(v, \xi, \varepsilon) = \eta_0(v, \xi) + \varepsilon \eta_1(v, \xi) + O(\varepsilon^2), \\ \frac{dv}{d\tau} &= V(v, \varepsilon) = V_0(v) + \varepsilon V_1(v) + O(\varepsilon^2). \end{aligned} \quad (8)$$

The coefficient δ will be found also as asymptotical expansion

$$\delta = \delta_0(1 + \varepsilon\delta_1) + O(\varepsilon^2) . \quad (9)$$

Taking into account (8) we obtain for (6)

$$\begin{aligned} \varepsilon \frac{\partial \theta}{\partial v} V &= \eta(1 - \eta)e^\theta + \frac{1}{\delta} \frac{\partial^2 \theta}{\partial \xi^2}, \\ \varepsilon \frac{\partial \eta}{\partial v} V &= \varepsilon \eta(1 - \eta)e^\theta + \frac{1}{\varrho} \frac{\partial^2 \eta}{\partial \xi^2}. \end{aligned} \quad (10)$$

The problem for zero order approximation of the integral manifold (8) is derived from (10) under $\varepsilon = 0$:

$$\begin{aligned} \frac{\partial^2 \theta_0}{\partial \xi^2} + \delta_0 \eta_0(1 - \eta_0) e^{\theta_0} &= 0, \\ \frac{1}{\varrho} \frac{\partial^2 \eta_0}{\partial \xi^2} &= 0, \end{aligned} \quad (11)$$

with boundary conditions

$$\left. \frac{\partial \theta_0}{\partial \xi} \right|_{\xi=0} = 0, \quad \theta_0 \Big|_{\xi=1} = 0, \quad (12)$$

$$\left. \frac{\partial \eta_0}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \frac{\partial \eta_0}{\partial \xi} \right|_{\xi=1} = 0. \quad (13)$$

The second equation in (11) with boundary conditions (13) has the solution $\eta_0 = \eta_0(v)$. It is convenient to choose parameter v as $\eta_0(v, \xi) \equiv v$.

Thus, the first equation in (11) takes the form

$$\frac{\partial^2 \theta_0}{\partial \xi^2} + \delta_0 v(1 - v) e^{\theta_0} = 0 . \quad (14)$$

Consider the auxiliary boundary value problem

$$\begin{aligned} y'' + ae^y &= 0 , \\ y'(0) = y(1) &= 0 . \end{aligned} \quad (15)$$

The solution of (15) is

$$y = 2(\ln \operatorname{ch} \sigma - \ln \operatorname{ch} \sigma \xi) , \quad (16)$$

where σ is the solution of transcendental equation

$$\operatorname{ch}(\sigma) = \sqrt{\frac{2}{a}} \sigma . \quad (17)$$

Under some $a = a^*$ the last equation possesses the unique solution $\sigma = \sigma^*$, under $a > a^*$ there are no solutions, and under $a < a^*$ there are two solutions of this equation. The corresponding approximate values for a^* and σ^* are

$$a^* = 0.878457, \quad \sigma^* = 1.19968. \quad (18)$$

It is clear that the boundary value problems (16), (12) and (14), (12) are coincident under $a = \delta_0 v(1-v)$. The maximal value of the right-hand side of last equality is $\delta_0/4$ under $v = 1/2$. The zero approximation of the critical value of the coefficient δ is thus seen to be $4a^*$, and for δ_0 we obtain the approximate value

$$\delta_0 = 4a^* = 3.513828. \quad (19)$$

By this means under the condition $\delta_0 < \delta_0^*$ the boundary value problem (14), (12) possesses two solutions. Upper solution corresponding to high temperatures is unstable, and lower one is stable. The solutions coincide at the point $v = 1/2$ under the condition $\delta_0 = \delta_0^*$, and under the condition $\delta_0 > \delta_0^*$ there exists such interval (v_1, v_2) that there are no solutions on it. The following expressions as a zero order approximation for the slow one-dimensional integral manifold are obtained:

$$\theta = \theta_0(v, \xi), \quad \eta = v,$$

where θ_0 is a chosen solution of the boundary value problem (14), (12) under the condition $\delta_0 = \delta_0^*$.

Substituting (8), (9) in (6), (7) and equating coefficients at ε we obtain the problem for the first order approximation

$$\begin{aligned} \frac{\partial^2 \theta_1}{\partial \xi^2} + \delta_0 v(1-v)e^{\theta_0} \theta_1 &= \delta_0 \left(\frac{\partial \theta_0}{\partial v} V_0 - (1-2v)e^{\theta_0} \eta_1 - \delta_1 v(1-v)e^{\theta_0} \right), \\ \frac{\partial^2 \eta_1}{\partial \xi^2} + v(1-v)e^{\theta_0} &= V_0, \end{aligned} \quad (20)$$

with the boundary conditions

$$\left. \frac{\partial \theta_1}{\partial \xi} \right|_{\xi=0} = 0, \quad \theta_1 \Big|_{\xi=1} = 0. \quad (21)$$

$$\left. \frac{\partial \eta_1}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \frac{\partial \eta_1}{\partial \xi} \right|_{\xi=1} = 0. \quad (22)$$

Integrating (20) over ξ from 0 to 1 and taking into account (22) we obtain

$$V_0 = v(1-v) \int_0^1 e^{\theta_0(\xi,v)} d\xi. \quad (23)$$

To calculate the integral in (23) we use (16) and get

$$\theta_0(\xi, v) = 2 \ln \operatorname{ch}(\sigma(v)) - 2 \ln \operatorname{ch}(\sigma(v)\xi) , \quad (24)$$

where $\sigma(v)$ is the solution of (17) under $a = v(1-v)\delta_0$ and, therefore,

$$e^{\theta_0(\xi,v)} = \frac{\operatorname{ch}^2(\sigma(v))}{\operatorname{ch}^2(\sigma(v)\xi)} . \quad (25)$$

From the last formula we have

$$\begin{aligned} V_0(v) &= v(1-v) \int_0^1 \frac{\operatorname{ch}^2(\sigma(v))}{\operatorname{ch}^2(\sigma(v)\xi)} d\xi = v(1-v) \frac{\operatorname{ch}^2(\sigma(v))}{\sigma(v)} \operatorname{th}(\sigma(v)) = \\ &= v(1-v) \left(\frac{\operatorname{ch}(\sigma(v))}{\sigma(v)} \right)^2 \sigma(v) \operatorname{th}(\sigma(v)) . \end{aligned} \quad (26)$$

It should be noted that under $\nu = 1/2$ taking into account the identity

$$1 - \sigma^* \operatorname{th}(\sigma^*) = 0 , \quad (27)$$

from (17) we obtain

$$V_0\left(\frac{1}{2}\right) = \frac{1}{4} \left(\frac{\operatorname{ch}(\sigma^*)}{\sigma^*} \right)^2 \sigma^* \operatorname{th}(\sigma^*) = \frac{1}{4} \frac{2}{a^*} = \frac{2}{\delta_0^*} . \quad (28)$$

To define the first order approximation of the critical value of the parameter δ we consider the first equation (20) under the condition $v = 1/2$ and obtain

$$\begin{aligned} \frac{\partial^2 \theta_1}{\partial \xi^2} + \frac{\delta_0}{4} e^{\theta_0} \theta_1 &= f(\xi) , \\ f(\xi) &= \delta_0 \left(\frac{\partial \theta_0(\xi, \frac{1}{2})}{\partial v} V_0\left(\frac{1}{2}\right) - \frac{\delta_1}{4} e^{\theta_0(\xi, \frac{1}{2})} \right) . \end{aligned} \quad (29)$$

The corresponding homogeneous boundary value problem

$$\begin{aligned} \frac{\partial^2 \theta_1}{\partial \xi^2} + \frac{\delta_0}{4} e^{\theta_0} \theta_1 &= 0 , \\ \frac{\partial \theta_1}{\partial \xi} \Big|_{\xi=0} = \theta_1 \Big|_{\xi=0} &= 0 , \end{aligned} \quad (30)$$

has nontrivial solution $\varphi_0(\xi)$, which is an eigenfunction corresponding to zero eigenvalue:

$$\varphi_0(\xi) = 1 - \sigma^* \xi \operatorname{th}(\sigma^* \xi) . \quad (31)$$

Thus, the solvability condition for the boundary value problem (29) is

$$\int_0^1 f(\xi) \varphi_0(\xi) d\xi = 0 \quad (32)$$

or

$$\int_0^1 \left(\frac{\partial \theta_0(\xi, \frac{1}{2})}{\partial v} V_0\left(\frac{1}{2}\right) - \frac{\delta_1}{4} e^{\theta_0(\xi, \frac{1}{2})} \right) (1 - \sigma^* \xi \operatorname{th}(\sigma^* \xi)) d\xi = 0 . \quad (33)$$

Note that (33) exactly coincides with the condition (??) of continuity of integral manifold at the point $v = 1/2$ (.2.2).

Let us calculate now functions contained in (33). Formula (24) implies

$$\frac{\partial \theta_0}{\partial v} = 2(\operatorname{th}(\sigma(v)) - \operatorname{th}(\sigma(v)\xi)) \frac{\partial \sigma}{\partial v} . \quad (34)$$

It is convenient to rewrite (17) in the form

$$\frac{\operatorname{ch}(\sigma)}{\sigma} = \sqrt{\frac{2}{\delta_0}}, [v(1-v)]^{-\frac{1}{2}} . \quad (35)$$

Differentiating (34) with respect to v we obtain

$$\left(\frac{\operatorname{sh}(\sigma)}{\sigma} - \frac{\operatorname{ch}(\sigma)}{\sigma^2} \right) \frac{\partial \sigma}{\partial v} = -\frac{1}{2} \sqrt{\frac{2}{\delta_0}}, [v(1-v)]^{-\frac{3}{2}} (1-2v) . \quad (36)$$

Taking into consideration that under $\nu = 1/2$ the equalities

$$\frac{\operatorname{sh}(\sigma)}{\sigma} - \frac{\operatorname{ch}(\sigma)}{\sigma^2} = 0, \quad 1 - 2v = 0 , \quad (37)$$

hold, and after iterated differentiation, we obtain under $v = 1/2$

$$\left(\frac{\operatorname{ch}(\sigma^*)}{\sigma^*} - \frac{\operatorname{sh}(\sigma^*)}{\sigma^{*2}} + 2 \frac{\operatorname{ch}(\sigma)}{\sigma^{*3}} \right) \left(\frac{\partial \sigma}{\partial v} \right)^2 \Big|_{v=\frac{1}{2}} = \sqrt{\frac{2}{\delta_0}} [v(1-v)]^{-\frac{3}{2}} \Big|_{v=\frac{1}{2}} . \quad (38)$$

The last expression may be simplified to the form

$$\begin{aligned} \frac{\operatorname{ch}(\sigma^*)}{\sigma^*} - \frac{\operatorname{sh}(\sigma^*)}{\sigma^{*2}} + 2 \frac{\operatorname{ch}(\sigma)}{\sigma^{*3}} &= \\ &= \frac{\operatorname{ch}(\sigma^*)}{\sigma^*} + 2 \frac{\operatorname{ch}(\sigma)}{\sigma^{*3}} (1 - \sigma^* \operatorname{th}(\sigma^*)) = \frac{\operatorname{ch}(\sigma^*)}{\sigma^*} . \end{aligned} \quad (39)$$

By virtue of (35) equation (38) takes the form

$$\left(\frac{\partial\sigma}{\partial v}\right)^2 \Big|_{v=\frac{1}{2}} = [v(1-v)]^{-1} \Big|_{v=\frac{1}{2}} = 4 \quad (40)$$

or

$$\frac{\partial\sigma}{\partial v} \Big|_{v=\frac{1}{2}} = \pm 2. \quad (41)$$

Consequently, we obtain

$$\frac{\partial\theta_0}{\partial v} \Big|_{v=\frac{1}{2}} = \pm 4(\text{th}(\sigma^*) - \xi \text{th}(\sigma^*\xi)) = \pm \frac{4}{\sigma^*}(1 - \sigma^*\xi \text{th}(\sigma^*\xi)), \quad (42)$$

Note that the sign ”+” corresponds to the transfer from the stable part of slow curve to unstable one and the sign ”-” corresponds to transfer from the unstable part to the stable one. Hence, trajectories that passed at first along the stable part and after that – along the unstable part (canards) correspond to the positive value $(\partial\theta_0/\partial v)|_{v=1/2}$.

It follows from (33) that

$$\begin{aligned} \delta_1 &= 4 \frac{\int_0^1 \frac{\partial\theta_0(\xi, \frac{1}{2})}{\partial v} V_0\left(\frac{1}{2}\right) (1 - \sigma^*\xi \text{th}(\sigma^*\xi)) d\xi}{\int_0^1 \frac{\text{ch}^2(\sigma^*)}{\text{ch}^2(\sigma^*\xi)} (1 - \sigma^*\xi \text{th}(\sigma^*\xi)) d\xi} = \\ &= \pm \frac{32}{\delta_0^* \sigma^*} \frac{\int_0^1 (1 - \sigma^*\xi \text{th}(\sigma^*\xi))^2 d\xi}{\int_0^1 \frac{\text{ch}^2(\sigma^*)}{\text{ch}^2(\sigma^*\xi)} (1 - \sigma^*\xi \text{th}(\sigma^*\xi)) d\xi} \simeq \pm 2.22. \end{aligned} \quad (43)$$

Thus

$$\delta^* = \delta_0(1 + \delta_1\varepsilon + O(\varepsilon^2)) \quad (44)$$

corresponds to a canard and gives the required critical condition for a thermal explosion (first limit of self-ignition). The value

$$\delta^{**} = \delta_0(1 - \delta_1\varepsilon + O(\varepsilon^2)) \quad (45)$$

corresponds to the false canard and gives the second limit of self-ignition. The interval (δ^*, δ^{**}) corresponds to transitional regimes of combustion. For the difference of the values δ^* and δ^{**} we have

$$\delta^* - \delta^{**} = 2\delta_0\delta_1\varepsilon + O(\varepsilon^2) \simeq 15.58\varepsilon + O(\varepsilon^2) \quad (46)$$

For the first order reaction one may use the generalization of the algorithm, worked out in [7], but in this case it may be applied in the numerical form only. Thus, for $\rho = 1$ we have at $\varepsilon = 0.01$ the value of $\delta = 1.02$, and at $\varepsilon = 0.02$ the value of $\delta = 0.98$.

4 Critical conditions of cylindrical reactor

Now, we put $n = 1$ in (1)–(2) and investigate the critical conditions of thermal explosion for the cylindrical reactor. In doing so, we have

$$\begin{aligned} \varepsilon \frac{\partial \theta}{\partial \tau} &= \eta(1 - \eta) e^\theta + \frac{1}{\delta} \left(\frac{\partial^2 \theta}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \theta}{\partial \xi} \right), \\ \varepsilon \frac{\partial \eta}{\partial \tau} &= \varepsilon \eta(1 - \eta) e^\theta + \frac{1}{\varrho} \left(\frac{\partial^2 \eta}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \eta}{\partial \xi} \right), \end{aligned} \quad (47)$$

with boundary conditions

$$\left. \frac{\partial \theta}{\partial \xi} \right|_{\xi=0} = \theta \Big|_{\xi=1} = 0, \quad \left. \frac{\partial \eta}{\partial \xi} \right|_{\xi=0} = \frac{\partial \eta}{\partial \xi} \Big|_{\xi=1} = 0. \quad (48)$$

In the same manner as in the previous Section, we try to find the slow one-dimensional stable-unstable integral manifold in a parametric form

$$\begin{aligned} \theta &= \theta(v, \xi, \varepsilon) = \theta_0(v, \xi) + \varepsilon \theta_1(v, \xi) + O(\varepsilon^2), \\ \eta &= \eta(v, \xi, \varepsilon) = \eta_0(v, \xi) + \varepsilon \eta_1(v, \xi) + O(\varepsilon^2), \\ \frac{dv}{d\tau} &= V(v, \varepsilon) = V_0(v) + \varepsilon V_1(v) + O(\varepsilon^2). \end{aligned} \quad (49)$$

The factor δ will be calculated as asymptotic expansion with respect to degrees of the small parameter ε :

$$\delta = \delta_0(1 + \varepsilon\delta_1) + O(\varepsilon^2). \quad (50)$$

Given (49), system (47) results in:

$$\begin{aligned} \varepsilon \frac{\partial \theta}{\partial v} V &= \eta(1 - \eta) e^\theta + \frac{1}{\delta} \left(\frac{\partial^2 \theta}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \theta}{\partial \xi} \right), \\ \varepsilon \frac{\partial \eta}{\partial v} V &= \varepsilon \eta(1 - \eta) e^\theta + \frac{1}{\varrho} \left(\frac{\partial^2 \eta}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \eta}{\partial \xi} \right), \end{aligned} \quad (51)$$

Setting $\varepsilon = 0$ in (10) we obtain the problem for the zero order approximation of the integral manifold (8):

$$\begin{aligned} \frac{\partial^2 \theta_0}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \theta_0}{\partial \xi} + \delta_0 \eta_0 (1 - \eta_0) e^{\theta_0} &= 0, \\ \frac{\partial^2 \eta_0}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \eta_0}{\partial \xi} &= 0, \end{aligned} \quad (52)$$

with boundary conditions

$$\left. \frac{\partial \theta_0}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \theta_0 \right|_{\xi=1} = 0. \quad (53)$$

$$\left. \frac{\partial \eta_0}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \frac{\partial \eta_0}{\partial \xi} \right|_{\xi=1} = 0. \quad (54)$$

Function $\eta_0 = \eta_0(v)$ is a solution of the second equation in (52) with boundary conditions (54). Since we have some freedom of choice of the parameter v , we put $\eta_0(v, \xi) \equiv v$.

The first equation in (52) takes the form

$$\frac{\partial^2 \theta_0}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \theta_0}{\partial \xi} + \delta_0 v (1 - v) e^{\theta_0} = 0. \quad (55)$$

Now, we consider an auxiliary problem

$$\begin{aligned} y'' + \frac{1}{\xi} y' + a e^y &= 0, \\ y'(0) = y(1) &= 0. \end{aligned} \quad (56)$$

It can be easily verified that function

$$y = 2 \ln \frac{2\sqrt{\frac{2}{a}} \left(\sqrt{\frac{2}{a}} \pm \sqrt{\frac{2}{a} - 1} \right)}{1 + \xi^2 \left(\sqrt{\frac{2}{a}} \pm \sqrt{\frac{2}{a} - 1} \right)^2} = 2 \ln \frac{2 \left(1 \pm \sqrt{1 - \frac{a}{2}} \right)}{\frac{a}{2} + \xi^2 \left(1 \pm \sqrt{1 - \frac{a}{2}} \right)^2} \quad (57)$$

is a solution to (56). Obviously, for $a = 2$ the last equation has a single solution, for $a > 2$ there are no solutions, and for $a < 2$ there are two solutions. Of these two solutions, the lower, corresponding to smaller temperatures, is stable, and the upper one is unstable.

Problems (56) and (52), (53) coincide at $a = \delta_0 v (1 - v)$. The greatest value of the right-hand side of this relation equals to $\delta_0/4$ for $v = 1/2$. That is why the critical value of coefficient δ equals to $4a^*$ in its zero order approximation, i. e., we obtain the approximate value for δ_0 :

$$\delta_0^* = 4a^* = 8. \quad (58)$$

Thus, for $\delta_0 > \delta_0^*$ system (55), (53) has no solutions, and for $\delta_0 = \delta_0^*$ there are two solutions

$$\theta_0^+(\xi, v) = 2 \ln \frac{2(1 + \sqrt{1 - 4v(1 - v)})}{4v(1 - v) + \xi^2(1 + \sqrt{1 - 4v(1 - v)})^2}, \quad (59)$$

$$\theta_0^-(\xi, v) = 2 \ln \frac{2(1 - \sqrt{1 - 4v(1 - v)})}{4v(1 - v) - \xi^2(1 + \sqrt{1 - 4v(1 - v)})^2}, \quad (60)$$

which stick together at the point $v = 1/2$; here θ_0^- is stable, and θ_0^+ is unstable. For $\delta_0 < \delta_0^*$ there are two solutions.

The following expressions are the zero order approximations for one-dimensional slow integral manifold:

$$\theta = \theta_0(v, \xi), \quad \eta = v,$$

where, as θ_0 , should be chosen one of solutions of boundary problem (55), (53), regarded for $\delta_0 = \delta_0^*$.

To obtain the problem for the first order approximation, we substitute (49), (49) into (47), (48) and equate the coefficients at ε :

$$\begin{aligned} \frac{\partial^2 \theta_1}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \theta_1}{\partial \xi} + \delta_0 v(1 - v) e^{\theta_0} \theta_1 &= \\ &= \delta_0 \left(\frac{\partial \theta_0}{\partial v} V_0 - (1 - 2v) e^{\theta_0} \eta_1 - \delta_1 v(1 - v) e^{\theta_0} \right), \end{aligned} \quad (61)$$

$$\frac{1}{\varrho} \left(\frac{\partial^2 \eta_1}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \eta_1}{\partial \xi} \right) + v(1 - v) e^{\theta_0} = V_0,$$

with boundary conditions

$$\left. \frac{\partial \theta_1}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \theta_1 \right|_{\xi=1} = 0. \quad (62)$$

$$\left. \frac{\partial \eta_1}{\partial \xi} \right|_{\xi=0} = 0, \quad \left. \frac{\partial \eta_1}{\partial \xi} \right|_{\xi=1} = 0. \quad (63)$$

Multiplying the second equation in (61) by ξ , integrating by ξ from 0 to 1, and taking into account (63), we derive

$$\int_0^1 \xi V_0 d\xi = v(1 - v) \int_0^1 \xi e^{\theta_0(\xi, v)} d\xi + \frac{1}{\varrho} \int_0^1 \frac{\partial}{\partial \xi} \left(\xi \frac{\partial \eta_1}{\partial \xi} \right) d\xi, \quad (64)$$

whence

$$\frac{1}{2} V_0 = v(1 - v) \int_0^1 \xi e^{\theta_0(\xi, v)} d\xi. \quad (65)$$

Now, we calculate the integral in the right-hand side of (65) for $v = 1/2$:

$$\int_0^1 \xi e^{2 \ln \frac{2}{1+\xi^2}} d\xi = \int_0^1 \xi \frac{4}{(1+\xi^2)^2} d\xi = -2 \frac{1}{1+\xi^2} \Big|_0^1 = 1. \quad (66)$$

Hence,

$$V_0\left(\frac{1}{2}\right) = 2 \cdot \frac{1}{4} = \frac{1}{2}. \quad (67)$$

For $v = 1/2$ the first equation in (61) is as follows:

$$\begin{aligned} \frac{\partial^2 \theta_1}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial \theta_1}{\partial \xi} + \frac{\delta_0}{4} e^{\theta_0(\xi, \frac{1}{2})} \theta_1 &= f(\xi), \\ f(\xi) &= \delta_0 \left(\frac{\partial \theta_0(\xi, \frac{1}{2})}{\partial v} V_0\left(\frac{1}{2}\right) - \frac{\delta_1}{4} e^{\theta_0(\xi, \frac{1}{2})} \right). \end{aligned} \quad (68)$$

Let us find $\partial \theta_0 / \partial v|_{v=1/2}$ ($\delta_0 = 8$).

$$\begin{aligned} \frac{1}{2} \theta_0(\xi, v) &= \ln(\alpha \pm \sqrt{\alpha^2 - 1}) - \ln(1 + \xi^2 (\alpha \pm \sqrt{\alpha^2 - 1})^2) + \ln 2\alpha, \\ \alpha &= \sqrt{\frac{2}{\delta_0}} [v(1-v)]^{-\frac{1}{2}} = \frac{1}{2} [v(1-v)]^{-\frac{1}{2}} \end{aligned} \quad (69)$$

Now, we differentiate the first equation in (69) by v :

$$\begin{aligned} \frac{1}{2} \frac{\partial \theta_0}{\partial v} &= \left\{ \frac{1}{\alpha} + \frac{1 \pm \frac{\alpha}{\sqrt{\alpha^2 - 1}}}{\alpha \pm \sqrt{\alpha^2 - 1}} - \frac{2\xi^2 (\alpha \pm \sqrt{\alpha^2 - 1}) \left(1 \pm \frac{\alpha}{\sqrt{\alpha^2 - 1}}\right)}{1 + \xi^2 (\alpha \pm \sqrt{\alpha^2 - 1})^2} \right\} \frac{\partial \alpha}{\partial v} = \\ &= \left\{ \frac{1}{\alpha} + \frac{\pm 1}{\sqrt{\alpha^2 - 1}} - \frac{\pm 2\xi^2 (\alpha \pm \sqrt{\alpha^2 - 1})^2}{(1 + \xi^2 (\alpha \pm \sqrt{\alpha^2 - 1})^2) (\sqrt{\alpha^2 - 1})} \right\} \frac{\partial \alpha}{\partial v}. \end{aligned} \quad (70)$$

For the sake of brevity, introduce the following denotations: $\kappa(\alpha) = \alpha \pm \sqrt{\alpha^2 - 1}$ ($\kappa(1) = 1$). After this, equality (70) is reformulated as follows:

$$\begin{aligned} \frac{1}{2} \frac{\partial \theta_0}{\partial v} &= \left\{ \frac{1}{\alpha} + \frac{\pm 1}{\sqrt{\alpha^2 - 1}} - \frac{\pm 2\kappa^2 \xi^2}{(1 + \kappa^2 \xi^2) (\sqrt{\alpha^2 - 1})} \right\} \frac{\partial \alpha}{\partial v} = \\ &= \left\{ \frac{\sqrt{\alpha^2 - 1}}{\alpha} \pm \frac{1 - \kappa^2 \xi^2}{1 + \kappa^2 \xi^2} \right\} \frac{1}{\sqrt{\alpha^2 - 1}} \frac{\partial \alpha}{\partial v}. \end{aligned} \quad (71)$$

Taking into consideration, that

$$\frac{\partial \alpha}{\partial v} = -\frac{1}{4} [v(1-v)]^{-\frac{3}{2}} (1-2v) = \frac{1}{4} (2v-1) [v(1-v)]^{-\frac{3}{2}}, \quad (72)$$

$$\frac{1}{\sqrt{\alpha^2 - 1}} = \frac{1}{\sqrt{\frac{1}{4v(1-v)} - 1}} = \frac{\sqrt{4v(1-v)}}{\sqrt{1-4v+v^2}} = \frac{2[v(1-v)]^{\frac{1}{2}}}{|2v-1|}, \quad (73)$$

we have for (71):

$$\begin{aligned} \frac{1}{2} \frac{\partial \theta_0}{\partial v} \Big|_{v=\frac{1}{2}} &= \pm \frac{1-\xi^2}{1+\xi^2} \left\{ \frac{1}{2v(1-v)} \cdot \frac{2v-1}{|2v-1|} \right\} \Big|_{v=\frac{1}{2}} = \pm 2 \frac{1-\xi^2}{1+\xi^2}, \\ \frac{\partial \theta_0}{\partial v} \Big|_{v=\frac{1}{2}} &= \pm 4 \frac{1-\xi^2}{1+\xi^2}. \end{aligned} \quad (74)$$

Here sign " + " corresponds to the duck-trajectory.

The homogeneous boundary problem (68), (62) has a nontrivial solution (i. e. an eigenfunction, corresponding to the zero eigenvalue)

$$\varphi_0(\xi) = \frac{1-\xi^2}{1+\xi^2}. \quad (75)$$

Hence, the solvability condition of nonhomogeneous boundary problem (68), (62) is as follows:

$$\int_0^1 f(\xi) \varphi_0(\xi) d\xi = 0 \quad (76)$$

or

$$\int_0^1 \left(\frac{\partial \theta_0(\xi, \frac{1}{2})}{\partial v} V_0\left(\frac{1}{2}\right) - \frac{\delta_1}{4} e^{\theta(\xi, \frac{1}{2})} \right) \left(\frac{1-\xi^2}{1+\xi^2} \right) d\xi = 0, \quad (77)$$

whence

$$\begin{aligned} \delta_1 &= \frac{4 \int_0^1 \frac{\partial \theta_0(\xi, \frac{1}{2})}{\partial v} V_0\left(\frac{1}{2}\right) \frac{1-\xi^2}{1+\xi^2} d\xi}{\int_0^1 e^{\theta(\xi, \frac{1}{2})} \frac{1-\xi^2}{1+\xi^2} d\xi} = \pm 8 \frac{\int_0^1 \left(\frac{1-\xi^2}{1+\xi^2} \right)^2 d\xi}{\int_0^1 \frac{4}{(1+\xi^2)^2} \frac{1-\xi^2}{1+\xi^2} d\xi} = \\ &= \pm 2 \frac{\int_0^1 \left(\frac{1-\xi^2}{1+\xi^2} \right)^2 d\xi}{\int_0^1 \frac{1-\xi^2}{(1+\xi^2)^3} d\xi} = \pm 16 \frac{4-\pi}{4+\pi} \simeq \pm 1.9232. \end{aligned} \quad (78)$$

After all, we have the following:

$$\delta^* = \delta_0(1 + \delta_1 \varepsilon + O(\varepsilon^2)) \quad (79)$$

corresponds to the duck-trajectory and gives a desired critical condition of thermal explosion, and the value

$$\delta^{**} = \delta_0(1 - \delta_1 \varepsilon + O(\varepsilon^2)) \quad (80)$$

corresponds to the second limit of selfignition.

For the difference $\delta^* - \delta^{**}$ we have

$$\delta^* - \delta^{**} = 2\delta_0\delta_1\varepsilon + O(\varepsilon^2) \simeq 30.77\varepsilon + O(\varepsilon^2). \quad (81)$$

As for the plane-parallel reactor, in the case of the first order reaction for the cylindrical reactor, one has to apply numerical algorithms. In doing so, for $\rho = 1$, we have, for example, the following values of δ : $\delta = 2.02$ for $\varepsilon = 0.01$, and $\delta = 2.33$ for $\varepsilon = 0.02$.

Acknowledgments

The author thanks V. A. Sobolev for helpful discussions and comments.

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