Calculation of critical conditions for the filtration combustion model

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Abstract

The paper is devoted to the study of the dynamic model of the autocatalytic combustion reaction in an inert medium with partial heat removal from the reaction phase to the environment. We pay particular attention to modelling of the critical regime, which is a kind of a watershed between the slow burning regimes and explosion modes. New algorithm for computing a critical value of the control parameter is presented.

Keywords: filtration combustion; thermal explosion; critical phenomena; singular perturbations; integral manifolds; canards

1. Introduction

In last few years there was an increase in researches concerning multiphase combustions systems. The results of the studies are widely used in the problems of safety of gas emissions, explosive dust clouds, mixture detonations, transportation and use of combustible and explosive substances.

In the present paper we consider a mathematical model of autocatalytic combustion reaction in a multiphase medium. The multiphase nature of the process arises from the existence of inert phase alongside with the reactant phase. The inert medium could correspond, for example, to a dusty medium or a porous matrix. We paid particular attention to the modelling of the critical regime that is kind of a watershed between the slow burning regimes and thermal explosions.

The main goal of the mathematical theory of thermal explosion [1-4] is to study the dynamics of the combustion process for a given dimensions of the reactor, thermophysical and kinetic characteristics, heat transfer coefficient. These characteristics correspond to parameters of the differential system, which is a mathematical model of the process. Under certain conditions of values of these parameters, the reaction proceeds for as long as possible without transition into the explosion or the slow burning mode. We call such regime a critical one.

The goal of the present work is to determine the values of the parameters that correspond to the critical regime. In order to find the values we consistently applied analytical and numerical methods. The main result of the paper is the derivation of the algorithm used in calculation of a value of the control parameter of the system that corresponds to the critical regime. The critical value of the control parameter is a solution of an algebra-differential system.

2. Model

We consider combustion model of a rarefied gas mixture in an inert porous, or in a dusty, medium. We assume that the temperature distribution and phase-to-phase heat exchange are uniform. The chemical conversion kinetics are represented by a one-stage, irreversible reaction. The dimensionless model in this case has the form [5-7]:

$$\gamma \frac{d\theta}{d\tau} = \eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right) - \alpha(\theta-\theta_c) - \delta\theta, \tag{1}$$

$$\gamma_c \frac{d\theta_c}{d\tau} = \alpha(\theta-\theta_c), \tag{2}$$

$$\frac{d\eta}{d\tau} = \eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right), \tag{3}$$

with initial condotions

$$\eta(0) = \eta_0/(1+\eta_0) = \bar{\eta}_0,\ \theta(0) = \theta_c(0) = 0. \tag{4}$$

Here θ and θ_c are the dimensionless temperatures of the reactant phase and of the inert phase, respectively; η is the depth of conversion; τ denotes the dimensionless time; η_0 is the parameter for autocatalyticity (this kinetic parameter characterizes the degree of self-acceleration of the reaction: the lower the value, the more marked the autocatalytic reaction will be). The terms $-\delta\theta$ and $-\alpha(\theta-\theta_c)$ reflect the external heat dissipation and phase-to-phase heat exchange. The parameters γ and γ_c characterize the physical features of the reactant phase and of the inert phase, respectively. System (1)-(3) is singularly perturbed since β and γ are the small for typical combustible gas mixture [1-3].

Depending on the relation between values of the parameters, the chemical reaction either moves to a slow regime with decay of the reaction, or into a regime of self-acceleration which leads to an explosion. So, if we change the value of one parameter, with fixed values of the other parameters, we can change the type of chemical reaction. Let us consider α as a control parameter. For some value of α (we call it critical) the reaction is maintained and gives rise to a rather sharp transition from slow motions to explosive ones. The transition region from slow regimes to explosive ones exists due to the continuous dependence of the system

(1)-(3) on the parameter α. To find the critical value of the parameter α, it is possible to use special asymptotic formulae [4, 7, 8]. That approach was used in [5-7, 9] for system (1)-(3), in [10-19] for other laser and chemical systems, and in [20-24] for some biological problems. In the next section the main results concerning this approach obtained for system (1)-(3) are given. The realizability conditions for the critical regime were obtained in the form of a system of non-linear algebra-differential equations, but the problem of calculating the critical value of the control parameter with the help of this system had not been solved. The paper is devoted to develop an algorithm for calculating the critical parameter value. The readers can find details of this algorithm in Sections 4 and 5.

3. Modelling of the critical regime

We will consider the case $\eta_0 = 0$ for the sake of simplicity, taking into account that for case $\eta_0 \neq 0$ the correction to the initial conditions can be found with help of fast integral manifolds [4].

The slow surface S of system (1)-(3) is described by the equation (see Figure 1):

$$\eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right) - \alpha(\theta-\theta_c) - \delta\theta = 0.$$

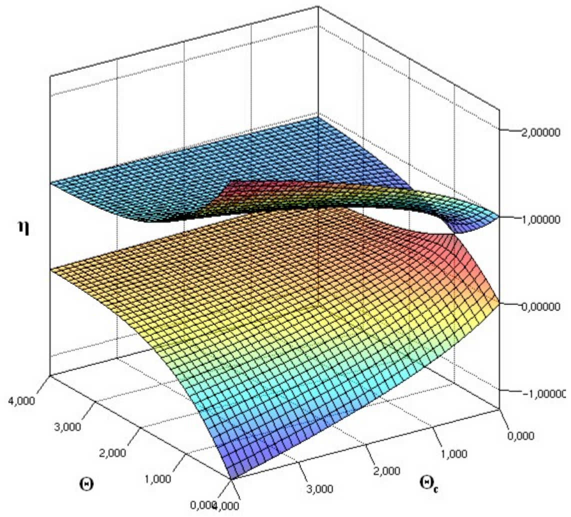

Fig. 1. The slow surface of system (1)-(3).

This surface is a zero-order (γ =0) approximation of a slow integral manifold of the system [4, 7, 8]. Recall, that the slow integral manifold of a singularly perturbed system is defined as an invariant surface of slow motions, i.e., the flow on it has the order $O(1)$ as $\gamma \to 0$. Far from the slow surface, the fast variables of the system vary very rapidly, with a speed of order $O(1/\gamma)$ as $\gamma \to 0$.

The intersection of the slow surface with the surface of irregular points (see Figure 2), given by the expression

$$\eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right)\frac{1}{(1+\beta\theta)^2} - \alpha - \delta = 0$$

determines a breakdown curve. The breakdown curve separates the stable (S^s) and unstable (S^u) subsets of the slow surface S, see Figure 3. System (1)-(3) has an stable integral manifold (S^s_ε) and an unstable integral manifold (S^u_ε) near S^s and S^u, respectively.

When $\alpha > \alpha^*$ the trajectories of the system starting at the initial point move along the stable branch S^s and the temperature θ does not reach relatively large values (see Figure 4). These trajectories correspond to the slow burning regimes.

When $\alpha < \alpha^*$ the system's trajectories, having reached the breakdown curve along S^s at the tempo of the slow variable, jump into the explosive regime (see Figure 5).

Due to the continuous dependence of the right-hand side of (1)-(3) on the parameter α there are some intermediate trajectories in the region between those shown above. For some value $\alpha = \alpha^*$ we can glue the stable and unstable slow integral manifolds at a point of the breakdown curve to get a canard [7, 8, 25, 26], i.e., the system's trajectory which at first move along the stable slow integral manifold and then continue for a while along the unstable slow integral manifold, see Figure 6.

The canard describes the critical regime that separates the domain of slow burning modes and the domain of thermal explosion. A deviation from the value of α^* leads to the destruction of the gluing of stable and unstable slow integral manifolds with a subsequent reaction's transition either to the slow regime (when the trajectory of the system unfolds along a stable manifold from the breakdown curve) or into the thermal explosion mode (when the trajectory, reaching the breakdown curve, jumps from the slow manifold and rapidly runs away from it).

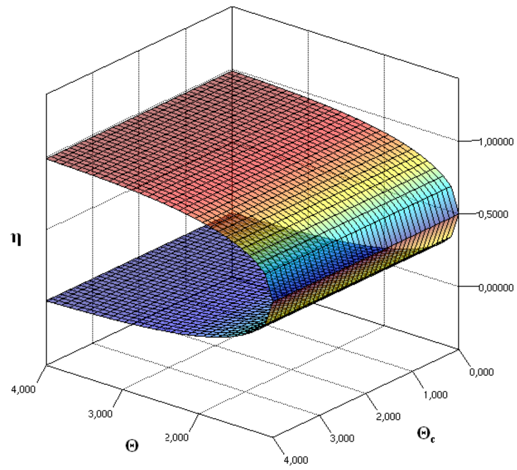

Fig. 2. The surface of irregular points.

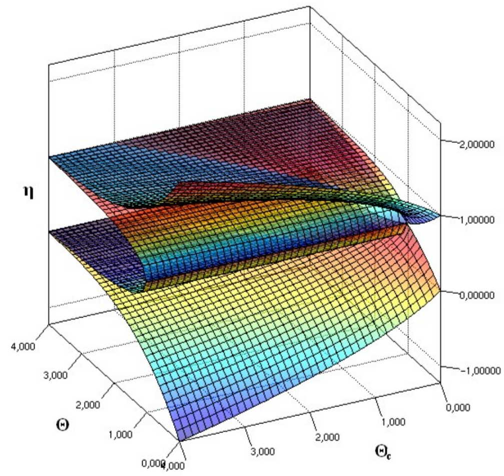

Fig. 3. The intersection of the slow surface of system (1)-(3) with the surface of irregular points. On the intersection (the breakdown line) the stability of the slow manifold changes. The upper and lower sheets of the slow surface are stable, the part enclosed between the surface of irregular points is unstable.

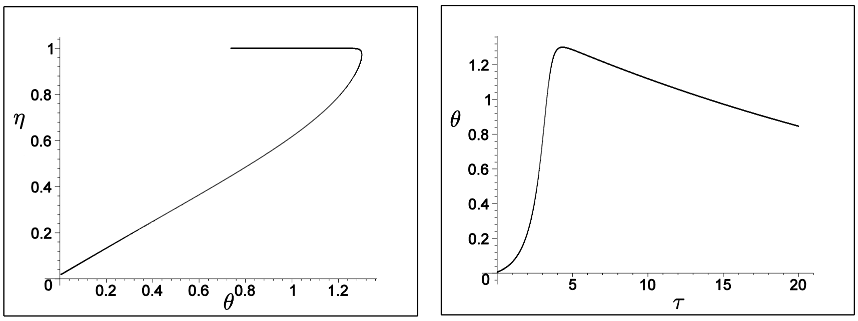

Fig. 4. The trajectory (left) and the θ-component (right) in the case of a slow birning regime: $\alpha = 3, \beta = 0.1, \gamma = 0.001, \gamma_c = 0.7, \bar{\eta}_0 = 0.02, \delta = 0.02$.

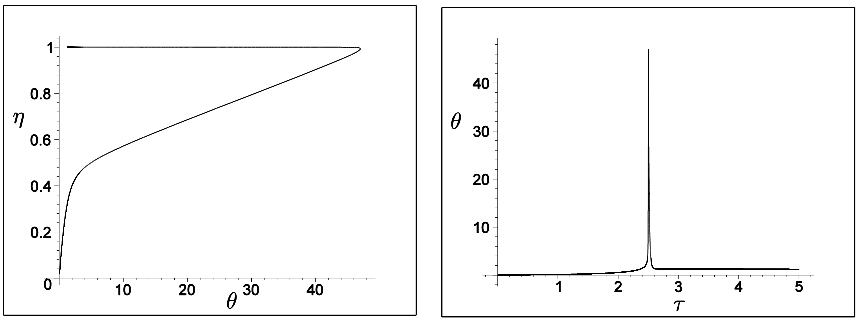

Fig. 5. trajectory (left) and the θ-component (right) in the case of thermal explosion: $\alpha = 0.7, \beta = 0.1, \gamma = 0.001, \gamma_c = 0.7, \bar{\eta}_0 = 0.02, \delta = 0.02$.

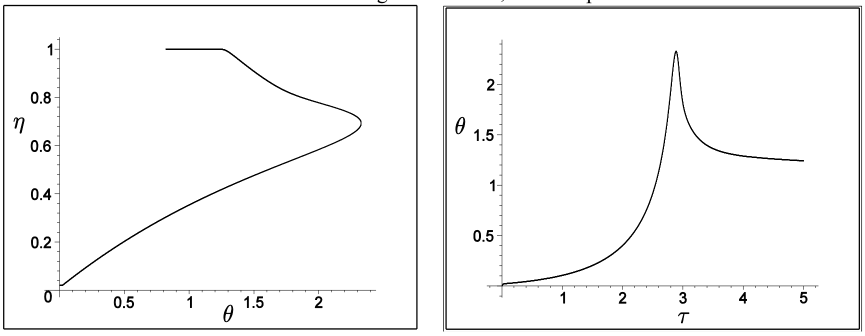

Fig. 6. The canard and the θ-component (right) in the case of critical regime: $\alpha = 0.949$, $\beta = 0.1$, $\gamma = 0.001$, $\gamma_c = 0.7$, $\bar{\eta}_0 = 0.02$, $\delta = 0.02$.

To calculate the critical value of the parameter $\alpha = \alpha^*$ and the asymptotic expressions for the corresponding canard

$$\alpha^* = \alpha_0 + \gamma\alpha_1 + o(\gamma),$$
$$\theta(\eta,\gamma) = \varphi_0(\eta) + \gamma\varphi_1(\eta) + o(\gamma), \tag{5}$$
$$\theta_c(\eta,\gamma) = \psi_0(\eta) + \gamma\psi_1(\eta) + o(\gamma),$$

we use the usual method of eliminating an independent variable. In this case, the system (1)-(3) takes the form

$$\gamma\frac{d\theta}{d\eta}\eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right) = \eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right) - \alpha(\theta-\theta_c) - \delta\theta,$$

$$\gamma_c\frac{d\theta_c}{d\eta}\eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right) = \alpha(\theta-\theta_c).$$

We substitute (5) into these equations to get

$$\gamma(\varphi_0' + \gamma\varphi_1')\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\left[1+\gamma\frac{\varphi_1}{(1+\beta\varphi_0)^2}\right] = \exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\left[1+\gamma\frac{\varphi_1}{(1+\beta\varphi_0)^2}\right]$$
$$-(\alpha_0+\gamma\alpha_1)\big(\varphi_0-\psi_0+\gamma(\varphi_1-\psi_1)\big) - \delta(\varphi_0+\gamma\psi_1) + o(\gamma), \tag{6}$$

$$\gamma_c(\varphi_0' + \gamma\varphi_1')\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\left[1+\gamma\frac{\varphi_1}{(1+\beta\varphi_0)^2}\right]$$
$$= (\alpha_0+\gamma\alpha_1)\big(\varphi_0-\psi_0+\gamma(\varphi_1-\psi_1)\big) + o(\gamma). \tag{7}$$

Setting $\gamma = 0$ in (6) and (7), we obtain

$$\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right) - \alpha_0(\varphi_0-\psi_0) - \delta\varphi_0 = 0, \tag{8}$$

$$\gamma_c\varphi_0'\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right) = \alpha_0(\varphi_0-\psi_0). \tag{9}$$

From the equation of the breakdown curve, taking into account (5), we have

$$\eta^*\,(1-\eta^*)\exp\left(\frac{\varphi_0^*}{1+\beta\varphi_0^*}\right)\frac{1}{(1+\beta\varphi_0^*)^2} - (\alpha_0+\delta) = 0, \tag{10}$$

where $(\eta^*, \varphi^*, \psi^*)$ is the gluing point of the slow integral manifolds.

After double differentiation (8) with respect to η, with taking into account (10), we get one more condition at the gluing point:

$$(1-2\eta^*)\exp\left(\frac{\varphi_0^*}{1+\beta\varphi_0^*}\right) + \alpha_0\psi_0'^* = 0,\;\; \psi_0'^* = \psi_0'(\eta^*). \tag{11}$$

Thus, the expressions (8)-(11) give us the zeroth order approximations of the critical value of the control parameter and the canard.

Further, in order to find the first order approximations, we equate the coefficients of γ in the first degree in the system (6), (7). As a result, we get:

$$\varphi_0\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right) = \left[\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\frac{\varphi_1}{(1+\beta\varphi_0)^2} - (\alpha_0+\delta)\right]\varphi_1 + \alpha_0\psi_1 - \alpha_1(\varphi_0-\psi_0), \tag{12}$$

$$\eta\,(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\left[\varphi_0'+\gamma_c\psi_1'+\frac{\varphi_1(\gamma_c\psi_0'-1)}{(1+\beta\varphi_0)^2}\right]=-\delta\varphi_1. \qquad (13)$$

$$\alpha_1=\frac{1}{\varphi_0^*-\psi_0^*}\left[\alpha_0\psi_1'^*-\varphi_0'^*\eta^*\,(1-\eta^*)\exp\left(\frac{\varphi_0^*}{1+\beta\varphi_0^*}\right)\right]. \qquad (14)$$

Here $\varphi_0'^*=\varphi_0'(\eta^*)$.

The expressions (12)-(14) determine the first order approximations of the critical value of the control parameter and the canard. It should be noted that to calculate the values of α_0 and α_1 from (8)-(14) it is necessary to apply numerical methods. The development of the algorithm for finding the critical value of the control parameter is our next goal.

4. The gluing point

In order to verify the correctness of the algorithm, developed in the present paper, we can use some specific case when an analytical solution of (8)-(14) is available and compare it to the one yielded by our method. For this goal we now consider the case δ =0 which corresponds the absence of external heat dissipation.

In the case δ =0 system (1)-(3) possesses a first integral

$$\eta-\gamma\theta-\gamma_c\,\theta_c\ =0.$$

With the help of this first integral, we can reduce the order of system (1)-(3) by eliminating the variable θ_c. As a result we obtain a plane system:

$$\gamma\frac{d\theta}{d\tau}=\eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right)-\alpha(1+\gamma/\gamma_c)\theta+\alpha/\gamma_c(\eta-\bar{\eta}_0),$$
$$\frac{d\eta}{d\tau}=\eta\,(1-\eta)\exp\left(\frac{\theta}{1+\beta\theta}\right).$$

Here we have to deal with the slow curve rather than then slow surface [5-7, 9]. The coordinates of the gluing point of the integral manifolds for some value $\alpha=\alpha_0$ can be found from the self-intersection conditions of the slow curve, which in our case have the form

$$\eta^*(1-\eta^*)\exp\left(\frac{\theta^*}{1+\beta\theta^*}\right)-\alpha\theta^*+\frac{\alpha}{\gamma_c}\eta^*=0, \qquad (15)$$
$$(1-2\eta^*)\exp\left(\frac{\theta^*}{1+\beta\theta^*}\right)+\frac{\alpha}{\gamma_c}=0, \qquad (16)$$
$$\eta^*(1-\eta^*)\exp\left(\frac{\theta^*}{1+\beta\theta^*}\right)\frac{1}{(1+\beta\theta^*)^2}-\alpha=0. \qquad (17)$$

From (15) and (17) we get

$$\eta^*=\gamma_c\theta^*-(1+\beta\theta^*)^2\gamma_c. \qquad (18)$$

Using (15) and (16), we obtain

$$(1-2\eta^*)(\theta^*-\gamma_c^{-1}\eta^*)+\gamma_c^{-1}\eta^*(1-\eta^*)=0.$$

From here it follows that

$$\gamma_c(1+\beta\theta^*)^4=\gamma_c\theta^{*2}-\theta^*. \qquad (19)$$

Equations (18) and (19) give us the values θ^* and η^*. Further, from equation (16) we obtain

$$\alpha_0=\gamma_c(2\eta^*-1)\exp\left(\frac{\theta^*}{1+\beta\theta^*}\right).$$

Using the smallness of the parameter β, from (19) we can analytically find the value θ^* in the form of an asymptotic expansion with respect to the parameter β: $\theta^*=\theta_{00}^*+\beta\theta_{01}^*+o(\beta)$. Similar expansions can also be written for α_0 and η^*. In the case $\beta=0$ we have:

$$\theta_{00}^*=\frac{1}{2}(\gamma_c^{-1}+\sqrt{4+\gamma_c^{-2}}),$$

$$\eta_{00}^*=\gamma_c(\theta_{00}^*-1),$$

$$\alpha_{00}=\frac{\exp(\theta_{00}^*)}{2+\sqrt{4+\gamma_c^{-2}}}.$$

5. Algorithm for calculating the critical value of the control parameter

Let us describe an algorithm for solving the system of nonlinear algebra-differential equations (8)–(11) with initial conditions that we obtained from (4)–(5):

$$\eta(0) = \frac{\eta_0}{1+\eta_0} = \bar{\eta}_0,\ \varphi_0(0) = \varphi_0.$$

We consider numerical solution of the system. Using (8) we get:

$$\psi_0 = \varphi_0\left(1 + \frac{\delta}{\alpha_0}\right) - \frac{\eta(1-\eta)}{\alpha_0}\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right).$$

Taking the derivative yields:

$$\psi_0' = \frac{1}{\alpha_0}\left[\varphi_0'(\alpha_0 + \delta) + (1 - 2\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right) - \eta(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\frac{\varphi_0'}{(1+\beta\varphi_0)^2}\right].$$

Now, let us substitute ψ_0 and ψ_0' into (9):

$$\varphi_0' = \left(\frac{\alpha_0}{\gamma_c} - \frac{\alpha_0\delta\varphi_0}{\gamma_c\eta(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)} + \frac{(1-2\eta)}{\eta(1-\eta)}\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)\right) \Big/ \left(\alpha_0 + \delta - \frac{\eta(1-\eta)\exp\left(\frac{\varphi_0}{1+\beta\varphi_0}\right)}{(1+\beta\varphi_0)^2}\right).$$

We get a first order ordinary differential equation with respect to $\varphi_0 = \varphi_0(\eta)$, where η is a variable and α_0 is a constant.

For any given value of α_0 we can solve the equation using Runge-Kutta fourth-order method. This method has a good precision and, in spite of its laboriousness, is widely used to obtain a numerical solution for ordinary differential equations. Moreover, we can further benefit from this method by using an adaptive stepsize.

Next, in order to the coordinates of the gluing point we find η^* and φ_0^* from (10) and (11):

$$\eta^*(1-\eta^*)\ \exp\left(\frac{{\varphi_0}^*}{1+\beta{\varphi_0}^*}\right)\frac{1}{(1+\beta\varphi_0^*)^2} - (\alpha_0 + \delta) = 0,$$

$$(1 - 2\eta^*)\exp\left(\frac{{\varphi_0}^*}{1+\beta{\varphi_0}^*}\right) + \alpha_0\frac{\eta^*(1-\eta^*)\ \exp\left(\frac{{\varphi_0}^*}{1+\beta{\varphi_0}^*}\right) - \delta{\varphi_0}^*}{\gamma_c\eta^*(1-\eta^*)\ \exp\left(\frac{{\varphi_0}^*}{1+\beta{\varphi_0}^*}\right)} = 0.$$

We can also solve this nonlinear system numerically using any of existing iterative methods. Let us note that sometimes it is possible to solve such systems by applying the elimination and back substitution method. However, in vast majority of cases iterative methods are used. Next, we substitute the solution η^* into (8) to obtain φ_0^{**}. Minimizing the difference between φ_0^* and φ_0^{**}, we can find α_0 with arbitrary precision.

Analogously, we get α_1 from (12)-(14) as we already computed α_0.

The algorithm was implemented using Java. To verify the correctness of the algorithm we considered a special case ($\beta = 0$, $\gamma = 0, \delta = 0$), that allows us to solve the system analytically. Then we compared the analytical solution with the numerical solution yielded by the algorithm. The results for α_0 are presented in Table 1.

Table 1. The comparison between analytical and numerical solutions for α_0 for various values of γ_c.

	α_0	
γ_c	Analytical solution	Numerical solution
0.6	1.837200	1.837291
0.7	1.566012	1.566038
0.8	1.393921	1.393923
0.9	1.275978	1.275919
1.1	1.125980	1.125923
1.2	1.075605	1.075623
1.3	1.035258	1.035253

6. Conclusion

We have studied the mathematical model of filtration combustion of combustible gas in an autocatalytic reaction case. We have shown that the critical phenomena of the model can be described by the canard. The critical regime is a kind of watershed between the safe processes and thermal explosion regimes. We have established that it is possible to control the mode and, therefore, the combustion process by adjusting the parameter characterizing the heat removal from the reaction phase to the external environment.

We have developed a new algorithm that allows to compute the critical value of the control parameter by combining analytical methods of the geometric theory of singular perturbations and numerical methods. The presented algorithm can be used in other similar problems for studying critical phenomena in dynamic systems and calculating critical values of control parameters.

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