Maximal combustion temperature estimation

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Abstract. This work is concerned with the phenomenon of delayed loss of stability and the estimation of the maximal temperature of safe combustion. Using the qualitative theory of singular perturbations and canard techniques we determine the maximal temperature on the trajectories located in the transition region between the slow combustion regime and the explosive one. This approach is used to estimate the maximal temperature of safe combustion in multi-phase combustion models.

1. Introduction and physical background
We consider a model of combustion of a rarefied gas mixture in an inert, porous or 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 the case of an autocatalytic reaction has the form [14]

\[ \gamma \frac{d\theta}{d\tau} = \eta(1 - \eta) \exp(\theta / (1 + \beta \theta)) - \alpha(\theta - \theta_c), \]

\[ \gamma_c \frac{d\theta_c}{d\tau} = \alpha(\theta - \theta_c), \]

\[ \frac{d\eta}{d\tau} = \eta(1 - \eta) \exp(\theta / (1 + \beta \theta)), \]

with the initial conditions

\[ \eta(0) = \tilde{\eta}_0 / (1 + \tilde{\eta}_0) = \eta_0, \quad \theta(0) = \theta_c(0) = 0. \]

Here, \( \theta \) and \( \theta_c \) are the dimensionless temperatures of the reactant and inert phases, respectively; \( \eta \) is the depth of conversion; \( \tilde{\eta}_0 \) is the criterion for autocatalyticity; the dimensionless parameters \( \beta \) and \( \gamma \) characterize the physical properties of a gas mixture. For real combustible gas mixtures typical values of the parameter \( \gamma \) and \( \beta \) are small [9, 17]. The term \( -\alpha(\theta - \theta_c) \) reflects the phase-to-phase heat exchange. The parameter \( \gamma_c \) characterizes the physical features of the inert phase. Depending on the relation between values of the parameters, the chemical reaction either changes to a slow regime with a decay of the reaction, or into a regime of self–acceleration that 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. Thus, it is possible to consider this problem as a special control problem.

Note, that the system (1)–(3) possesses a first integral
\( \gamma \theta + \gamma_c \theta_c - \eta = \eta_0, \)

and therefore we obtain on eliminating \( \theta_c \)

\[
\gamma \frac{d\theta}{d\tau} = \eta (1 - \eta) \exp \left( \frac{\theta}{1 + \beta \theta} \right) - \alpha \left( 1 + \frac{\gamma}{\gamma_c} \right) \theta + \frac{\alpha}{\gamma_c} (\eta - \eta_0),
\]

(4)

\[
\frac{d\eta}{d\tau} = \eta (1 - \eta) \exp \left( \frac{\theta}{1 + \beta \theta} \right),
\]

(5)

with initial conditions

\[
\eta(0) = \eta_0, \quad \theta(0) = 0.
\]

(6)

The chemically relevant phase space \( \Delta \) of the system is defined by \( \Delta := \{(\theta, \eta) \in \mathbb{R}^2 : \theta \geq 0, 0 \leq \eta \leq 1\} \). As \( \gamma \) is small (for highly exothermic chemical systems typical values of \( \gamma \) lie in the interval \((0.01, 0.1)\), see, for example, [4]), (4) and (5) represent a singularly perturbed system of autonomous differential equations [15, 16]. A qualitative investigation of this system can be found in [3, 10, 13, 14]. In what follows we recall the main results of these studies.

Consider initial value problem (4)–(6) in \( \Delta \) for \( \alpha > 0, \gamma > 0 \). There are two equilibria: the point \( P = (1 - \eta_0)/(\gamma + \gamma_c), 1) \) is a stable node, the point \( Q = (-\eta_0)/(\gamma + \gamma_c), 0) \) is a saddle, but only \( P \) belongs to \( \Delta \).

If we put \( \gamma = 0 \) in (4) we get the degenerate equation

\[
0 = \eta (1 - \eta) \exp \left( \frac{\theta}{1 + \beta \theta} \right) - \alpha \left( \theta - \frac{\eta - \eta_0}{\gamma_c} \right) = F(\eta, \theta, \alpha),
\]

(7)

which describes the slow curve \( S_\alpha \) of (4), (5) (see, for example, [10, 11]).

The subset \( S_\alpha^{s} \) (\( S_\alpha^{u} \)) of \( S_\alpha \) with

\[
\frac{\partial}{\partial \theta} F(\eta, \theta, \alpha) < 0 \quad (> 0)
\]

is called the attractive (repulsive) subset of \( S_\alpha \). A point \( A \) on \( S_\alpha \) in which \( \partial F/\partial \theta = 0 \) is called the breakdown point [5, 10, 12]. For \( \gamma \) sufficiently small, the system (4), (5) has an attractive slow invariant manifold \( S_{\alpha, \gamma}^{s} \) near \( S_\alpha \) and a repulsive slow invariant manifold \( S_{\alpha, \gamma}^{u} \) near \( S_\alpha \), respectively (see, for example, [12]).

We take \( \alpha \) as control parameter with fixed \( \gamma_c \). The point \( \theta = \theta_s, \eta = \eta_s \) is the self–intersection point of the slow curve at \( \alpha = \alpha_0 \). Here, \( \alpha = \alpha_0, \theta = \theta_s, \eta = \eta_s \) satisfy the system

\[
F(\eta, \theta, \alpha) = F_\eta(\eta, \theta, \alpha) = F_\theta(\eta, \theta, \alpha) = 0.
\]

(8)

The dependence of the slow curve \( S_\alpha \) on the relation between parameter values gives different forms, see Figure 1.

In the case \( \alpha > \alpha_0 \) each set \( S_\alpha^{s} \) and \( S_\alpha^{u} \) of \( S_\alpha \) consists of a single connected curve, see Figure 1(a). Hence the system has an attractive invariant manifold \( S_{\alpha, \gamma}^{s} \) and a repulsive invariant manifold \( S_{\alpha, \gamma}^{u} \) near \( S_\alpha^{s} \) and \( S_\alpha^{u} \), respectively.

Since the initial point \((0, \eta_0)\) belongs to the basin of attraction of the set \( S_\alpha^{s} \), after a short time the trajectory follows the attractive slow invariant manifold \( S_{\alpha, \gamma}^{s} \) and tends to the equilibrium \( P \) as \( \tau \) tends to \( \infty \). This behavior corresponds to the slow combustion regime with low temperatures, see Figure 2.

In the case \( \alpha < \alpha_0 \) each set \( S_\alpha^{s} \) and \( S_\alpha^{u} \) consists of two different components separated by breakdown points \( A_1 \) and \( A_2 \) with \( \theta = \theta_A \) (see Figure 1(b)) and for \( \gamma \) sufficiently small the system has local attractive invariant manifolds \( S_{\alpha, \gamma}^{s,i} \) (repulsive invariant manifolds \( S_{\alpha, \gamma}^{u,i} \) near
Figure 1. The trajectories (the solid line) of the system (4), (5) and the slow curve (the dashed line) for (a) $\alpha > \alpha_0$, (b) $\alpha < \alpha_0$, (c) $\alpha = \alpha_0$.

Figure 2. The trajectory of the system (4), (5) and the $\eta$– and $\theta$–components of the solution in the case of the slow combustion regime for $\alpha = 1.4$, $\beta = 0.1$, $\gamma = 0.01$, $\gamma_c = 0.7$, $\eta_0 = 0.02$. 
Figure 3. The trajectory of the system (4), (5) and the $\eta$– and $\theta$– components of the solution in the case of thermal explosion for $\alpha = 0.7$, $\beta = 0.1$, $\gamma = 0.01$, $\gamma_c = 1.1$, $\eta_0 = 0.02$.

Each component of $S_{\alpha,1}^s (S_{\alpha,1}^u)$, $i = 1, 2$. In that case, we have the following behavior of the solution of the initial value problem (4)–(6): after a short time, the solution will follow the component of $S_{\alpha,1}^s$ to breakdown point $A_1$. After this time, $\theta(\tau)$ will increase rapidly, but the solution remains inside $\Delta$ and ultimately tends to the stable equilibrium $P$. In contrast to the case $\alpha > \alpha_0$ where $\theta(\tau)$ behaves much like $\eta(\tau)$ (see Figure 2), now the temperature rises steeply under insignificant changes of $\eta(\tau)$ (see Figure 3). A drastic growth of the temperature under negligible changes of the concentration (or depth of conversion) of the gas mixture is the characteristic property of a dangerous phenomenon called thermal explosion in combustion theory [9].

The transition region from the slow combustion regime to the explosive one exists due to the continuous dependence of our system on the parameters $\alpha$ and $\gamma_c$ ($\gamma_c > 0$). For $\alpha = \alpha_0$ the slow curve has an intersection point $(\theta_s, \eta_s)$, separating four branches $S_{\alpha_0,1}^u$, $S_{\alpha_0,2}^u$, $i = 1, 2$, see Figure 1(c). According to (7) and (8), the branch $S_{\alpha_0,1}^s$ has the representation

$$S_{\alpha_0,1}^s := \{ (\theta, \eta) \in \Delta : \eta = \zeta_1^s(\theta), \ 0 \leq \theta \leq \theta_s \},$$

(9)

where

$$\zeta_1^s(\theta) = \frac{1}{2} \left[ 1 + \frac{\alpha_0}{\gamma_c} \exp \left( \frac{-\theta}{1 + \beta \theta} \right) - \sqrt{\left( 1 + \frac{\alpha_0}{\gamma_c} \exp \left( \frac{-\theta}{1 + \beta \theta} \right) \right)^2 - 4\alpha_0 \exp \left( \frac{-\theta}{1 + \beta \theta} \right) \left( \theta + \frac{\eta_0}{\gamma_c} \right) } \right].$$

If we denote by $\psi_1^s(\eta)$ the inverse function of $\zeta_1^s(\theta)$, then $S_{\alpha_0,1}^s$ can also be represented in the form

$$S_{\alpha_0,1}^s := \{ (\theta, \eta) \in \Delta : \theta = \psi_1^s(\eta), \ 0 \leq \eta \leq \eta_s \}.$$  

(10)

Similarly, the branch $S_{\alpha_0,2}^s$ can be represented as

$$S_{\alpha_0,2}^s := \{ (\theta, \eta) \in \Delta : \eta = \zeta_2^s(\theta), \ \theta \geq \theta_s \} = \{ (\theta, \eta) \in \Delta : \theta = \psi_2^s(\eta), \ \eta_s \leq \eta < 1 \},$$

(11)

where

$$\zeta_2^s(\theta) = \frac{1}{2} \left[ 1 + \frac{\alpha_0}{\gamma_c} \exp \left( \frac{-\theta}{1 + \beta \theta} \right) + \sqrt{\left( 1 + \frac{\alpha_0}{\gamma_c} \exp \left( \frac{-\theta}{1 + \beta \theta} \right) \right)^2 - 4\alpha_0 \exp \left( \frac{-\theta}{1 + \beta \theta} \right) \left( \theta + \frac{\eta_0}{\gamma_c} \right) } \right].$$
acceleration reactions, both cases the distances travelled are equations if it, at first, follows an attractive invariant manifold, and then a repulsive one. In [2, 10]. Recall that a canard is a trajectory of a singularly perturbed system of differential equations if it, at first, follows an attractive invariant manifold, and then a repulsive one. Using the method of integral manifolds and the canard techniques in [10], it is possible to find the critical value of the parameter that corresponds to a trajectory modelling the critical regime in the chemical system in the form of the asymptotic representation

$$\alpha = \alpha^*(\gamma) = \alpha_0 + \alpha_1 \gamma + \alpha_2 \gamma^2 + O(\gamma^3),$$

where

$$\alpha_0 = \gamma_c(2\eta_s - 1) \exp\left(-\frac{\theta_s}{1 + \beta \theta_s}\right).$$

Also (recall that $\beta$ is a small parameter)

$$\theta_s = \theta_{s0} + \beta \theta_{s1} + O(\beta^2),$$

where

$$\theta_{s0} = \frac{1}{2\gamma_c} \left(1 - 2\eta_0 + \sqrt{1 + 4\gamma_c^2}\right),$$

$$\theta_{s1} = \frac{(1 - 2\eta_0 + \sqrt{1 + 4\gamma_c^2})^3 - 2\gamma_c(\eta_0^2 - \eta_0)}{2\gamma_c^2 \sqrt{1 + 4\gamma_c^2}};$$

and

$$\eta_s = \eta_{s0} + \beta \eta_{s1} + O(\beta^2),$$

where

$$\eta_{s0} = \gamma_c \theta_{s0} - \gamma_c + \eta_0 = \frac{1}{2} \left(1 + \sqrt{1 + 4\gamma_c^2}\right) - \gamma_c,$$

$$\eta_{s1} = \gamma_c(\theta_{s1} - 2\theta_{s0}) = \frac{(1 - 2\eta_0 + \sqrt{1 + 4\gamma_c^2})^3 - 2\gamma_c(\eta_0^2 - \eta_0)}{2\gamma_c \sqrt{1 + 4\gamma_c^2}} - \left(1 - 2\eta_0 + \sqrt{1 + 4\gamma_c^2}\right).$$

This trajectory after a short time follows the attractive component $S_{\alpha_0}^{a,1}$ until it reaches the value $\theta = \theta_s$. After this moment, it stays near the repulsive component $S_{\alpha_0}^{u,2}$, up to a point $J$ from which the solution “jumps” towards the attractive component $S_{\alpha_0}^{a,2}$ and tends to $P$ as $\tau \to \infty$, see Figure 1(c).

This trajectory contains the attractive/repulsive part of slow motions and thus, is a canard [2, 10]. Recall that a canard is a trajectory of a singularly perturbed system of differential equations if it, at first, follows an attractive invariant manifold, and then a repulsive one. In both cases the distances travelled are $O(1)$ as $\gamma \to 0$.

The canard corresponds to a critical chemical reaction separating the domain of self-acceleration reactions ($\alpha < \alpha^*$) and the domain of non-explosive reactions ($\alpha > \alpha^*$). Note, that this regime is not a slow combustion regime since the temperature attains a high value, and is not explosive as the temperature increases at the tempo of the slow variable. Figure 4 shows the results of the numerical investigation of (4)–(6) for the case $\alpha = \alpha^*$.

The sufficient conditions for the existence and the algorithm for the construction of the canard solution of system (4), (5) were given in [14].

Thus, this fact is very important: during the critical regime the temperature attains a high value but without explosion, and this may be the aim of a technological process.

The problem of the location of critical regimes thought of as regimes separating the regions of explosive and nonexplosive chemical reactions is the significant mathematical problem of thermal
Figure 4. The trajectory of the system (4), (5) and the $\eta$– and $\theta$–components of the solution in the case of critical regime for $\alpha = \alpha^* = 0.949$, $\beta = 0.1$, $\gamma = 0.01$, $\gamma_c = 0.7$, $\eta_0 = 0.02$.

explosion theory. The interest in critical phenomena is occasioned by not only for reasons of safety, but in many cases the critical regime is the most effective in technological processes.

So, we are interested in the determination of the value of the maximal temperature during the critical regime as a maximal temperature of safe combustion. In other words, we are interested in the determination of the jump-off point $J$ (the point in which a trajectory modelling the critical regime jumps from the repulsive invariant manifold, see Figure 1(c)), and therefore the maximal temperature on a canard trajectory. To solve this problem we use an estimate of the delay of loss of stability in scalar singularly perturbed equations.

2. Delay of loss of stability in scalar non-autonomous differential equations

We consider the scalar singularly perturbed differential equation

$$\varepsilon \frac{du}{d\eta} = g(u, \eta, \varepsilon)$$

(12)

and study the initial value problem

$$u(\eta_0, \varepsilon) = u_0, \quad \eta \in I_\eta := \{\eta \in \mathbb{R} : \eta_0 < \eta < \eta_1\}$$

(13)

for sufficiently small $\varepsilon$.

If we set $\varepsilon = 0$ in (12) we get the degenerate equation

$$g(u, \eta, 0) = 0.$$

If this equation has a simple isolated root $u = \psi(\eta)$ which is a stable equilibrium of the associated equation

$$\frac{du}{d\tau} = g(u, \eta, 0),$$

(14)

and if $u_0$ belongs to region of attraction of $\psi(\eta_0)$, then the asymptotic behavior of the solution of the initial value problem (12), (13) is uniquely determined by the standard theory of singularly perturbed systems (see, e.g., [16]). In what follows we consider this initial value problem in the case of change of stabilities, that is, we assume that the degenerate equation has two intersecting solutions. Here, we have to distinguish two different situations: immediate loss of stability and
delayed loss of stability (see, for example [1, 6]). The latter case is related to the existence of a canard trajectory. We now recall a result concerning the delayed exchange of stabilities in the case of transversal bifurcation.

Let $U$ be an open bounded interval containing the origin, $I_{ε_0}$ is the open interval defined by $I_{ε_0} := \{ ε ∈ R : 0 < ε < ε_0, 0 < ε_0 ≤ 1 \}$.

We consider the initial value problem (12), (13) under the following assumptions:

$(A_1)$. $g : U × I_η × I_{ε_0} → R$ is continuous and twice continuously differentiable with respect to $u$ and $ε$.

$(A_2)$. $g(0, η, ε) ≡ 0$ for $(η, ε) ∈ I_η × I_{ε_0}$ (bar $I$ means the closure of $I$).

From $(A_1)$ and $(A_2)$ it follows that a solution of (12) starting at $u = u_0$ remains positive (negative) if $u_0$ is positive (negative). In the sequel we restrict ourselves to the case $u_0 < 0$. We denote by $U^−$ the set defined by $U^− := \{ u ∈ U : u ≤ 0 \}$.

$(A_3)$. The solution set of the degenerate equation $g(u, η, 0) = 0$ in $U^− × I_η$ consists of the two curves $u ≡ 0$ and $u = ψ^−(η)$ where $ψ^−$ belongs to the class $C^1([η_s, η_1], R^−)$ and satisfies $ψ^−(η_s) = 0, ψ^−(η) < 0$ for $η ∈ (η_s, η_1]$ (see Figure 5).

\[ G(η, η_0, ε) := \int_{η_0}^{η} g_u(0, η, ε) dξ. \]

From assumption $(A_4)$ we get that $G(η, η_0, 0) = 0$ has at most one root $η = η^*$ in $(η_0, η_1)$. Therefore, we assume

$(A_5)$. $G(η, η_0, 0) = 0$ has a root $η^*$ in $(η_0, η_1)$.

It is easy to see that $η^*$ is such that

\[ η^* > η_s, \quad G'(η^*, η_0, 0) > 0 \]

holds.

The following assumption on the function $g$ is satisfied if the second derivative of $g$ with respect to $u$ at $u = 0$ is positive for all $(η, ε)$ under consideration.

\[ \text{Figure 5. Solution set of } g(u, η, 0) = 0. \]
There are sufficiently small positive numbers $c_0$ and $\varepsilon_0$, such that \([-c_0, c_0] \subseteq U\) and

$$g(u, \eta, \varepsilon) \geq g_u(0, \eta, \varepsilon)u \quad \text{for} \quad \eta_0 \leq \eta \leq \eta^*, \quad \varepsilon \in T_{\varepsilon_0}, \quad -c_0 \leq u \leq 0.$$ 

The following result about the delayed exchange of stabilities has been proved in [7].

**Theorem.** Assume the hypotheses (A1) - (A6) to be valid. Then for sufficiently small $\varepsilon$ and $u_0 < 0$ there exists a unique solution of (12), (13) satisfying

$$\lim_{\varepsilon \to 0} u(\eta, \varepsilon) = \begin{cases} 
0 & \text{for } \eta \in [\eta_0, \eta^*), \\
\psi_-(\eta) & \text{for } \eta \in (\eta^*, \eta_*].
\end{cases}$$

After a short time the trajectory of this solution, starting from the initial point, first follows the $\eta$-axis until $\eta = \eta^*$. After this the trajectory jumps to the stable part of the curve $u = \psi_-(\eta)$, see Figure 6.

![Figure 6. Solution $u = u(\eta, \varepsilon)$ of (12), (13).](image)

3. Maximal temperature of safe combustion

We return to the combustion model.

Our goal is for $\alpha = \alpha^*(\gamma)$ and sufficiently small $\gamma$ to estimate the maximal temperature $\theta^\text{max}_\gamma$ on the canard trajectory of system (4), (5), which starts at the given initial point $(\eta = \eta_0, \theta = 0)$.

We apply the Theorem above to estimate the maximal temperature on the canard of the equation

$$\frac{d\theta}{d\eta} = \frac{\eta(1-\eta) \exp\left(\frac{\theta}{1+\beta\theta}\right) - \alpha^*(\gamma) \left(1 + \frac{\gamma}{\gamma_c}\right) \theta + \frac{\alpha^*(\gamma)}{\gamma_c} (\eta - \eta_0),}{\eta(1-\eta) \exp\left(\frac{\theta}{1+\beta\theta}\right)},$$

which follows from (4), (5) with $\alpha = \alpha^*(\gamma)$.

We use the coordinate transformation

$$\theta = \varphi(\eta, \eta_0, \varepsilon) + u,$$

where the function $\varphi(\eta, \eta_0, \varepsilon)$ describes the attractive/repulsive part of slow motions on the canard trajectory (near the attractive component $S_{\alpha_0}^{s,1}$ and the repulsive component $S_{\alpha_0}^{s,2}$, respectively), and

$$\varphi(\eta, \eta_0, \gamma) = \varphi_0(\eta, \eta_0) + \gamma \varphi_1(\eta, \eta_0) + \gamma^2 \varphi_2(\eta, \eta_0) + O(\gamma^3),$$

with

$$\varphi_0(\eta, \eta_0) = \begin{cases} 
\psi_1^s(\eta) & \text{for } 0 < \eta \leq \eta_s, \\
\psi_2^s(\eta) & \text{for } \eta_s \leq \eta < \eta^*.
\end{cases}$$
Here, \( \eta = \eta^* \) is a coordinate of the point \( J \) at which the canard jumps from the slow invariant manifold \( S_{u^*,2} \). Recall that this point characterizes the maximal temperature of safe combustion.

The coordinate transformation (16) permits us to rectify the attractive/repulsive part of the canard with slow motions. In the new variables the canard trajectory modelling the critical regime converts to the form which is shown on Figure 6.

Our aim is to calculate the value \( \eta^* \) using the Theorem.

From (15) applying the coordinate transformation (16) we get

\[
\frac{du}{d\eta} = \frac{\eta(1-\eta) \exp \left( \frac{\varphi + u}{1 + \beta \varphi + \beta u} \right) - \alpha^* (1 + \frac{\gamma}{\gamma_c}) \varphi - \frac{\alpha^*}{\gamma_c}(\eta - \eta_0) d\varphi}{\eta(1-\eta) \exp \left( \frac{\varphi + u}{1 + \beta \varphi + \beta u} \right) - \gamma d\eta}.
\]

The function \( \varphi = \varphi(\eta, \eta_0, \varepsilon) \) is a solution of equation (15). Hence, the last equation can be represented in the form

\[
\gamma \frac{du}{d\eta} = \frac{\alpha^*}{\eta(1-\eta)} \left( \left[ 1 + \frac{\gamma}{\gamma_c} \right] \varphi - \frac{\eta - \eta_0}{\gamma_c} \exp \left( \frac{-\varphi}{1 + \beta \varphi} \right) \right)
- \left[ \left( 1 + \frac{\gamma}{\gamma_c} \right) \left( \varphi + u \right) - \frac{\eta - \eta_0}{\gamma_c} \exp \left( \frac{-\varphi - u}{1 + \beta \varphi + \beta u} \right) \right] \equiv g(u, \eta, \gamma).
\]  

(18)

It is easy to verify that \( g(u, \eta, \gamma) \) satisfies all the assumptions of the Theorem for an appropriate choice of \( \eta_0 \) and \( \gamma \) sufficiently small.

According to (18) and the assumption (A5) of the Theorem, \( \eta^* \) is a root of the equation

\[
G(\eta, \eta_0, 0) = \int_{\eta_0}^{\eta} g_u(0, \xi, 0) d\xi = 0,
\]

where

\[
g_u(0, \eta, 0) = \frac{\alpha^*}{\eta(1-\eta)} \left[ \varphi_0 - \frac{\eta - \eta_0}{\gamma_c} \right] \frac{1}{(1 + \beta \varphi_0)^2} - 1 \exp \left( \frac{-\varphi_0}{1 + \beta \varphi_0} \right) = \frac{1}{(1 + \beta \varphi_0)^2} - \frac{\varphi_0 - \frac{\eta - \eta_0}{\gamma_c}}{1 + \beta \varphi_0}
\]

\[
\equiv \begin{cases} 
\frac{1}{(1 + \beta \psi_s^1(\eta))^2} - \frac{1}{\psi_s^1(\eta) - \frac{\eta - \eta_0}{\gamma_c}} & 0 < \eta < \eta_s, \\
\frac{1}{(1 + \beta \psi_s^2(\eta))^2} - \frac{1}{\psi_s^2(\eta) - \frac{\eta - \eta_0}{\gamma_c}} & \eta_s < \eta < \eta^*.
\end{cases}
\]

Hence,

\[
G(\eta, \eta_0, 0) = \int_{\eta_0}^{\eta_s} \left( \frac{1}{(1 + \beta \psi_s^1(\xi))^2} - \frac{1}{\psi_s^1(\xi) - \frac{\xi - \eta_0}{\gamma_c}} \right) d\xi
+ \int_{\eta_s}^{\eta} \left( \frac{1}{(1 + \beta \psi_s^2(\xi))^2} - \frac{1}{\psi_s^2(\xi) - \frac{\xi - \eta_0}{\gamma_c}} \right) d\xi.
\]

We have by (9)–(11)

\[
G(\eta, \eta_0, 0) = \int_{\theta_0}^{\theta_s} \left( \frac{1}{(1 + \beta \sigma)^2} - \frac{1}{\sigma - \frac{\eta_0}{\gamma_c}} \right) (\zeta_s^1)'(\sigma) d\sigma
\]
\[ + \int_{\theta_*}^{\theta} \left( \frac{1}{(1 + \beta \sigma)^2} - \frac{1}{\sigma - \frac{\zeta_2' \sigma - \eta_0}{\gamma c}} \right) \left( \zeta_2'' \right)'(\sigma) d\sigma \equiv \tilde{G}(\theta, \theta_0, 0). \] (19)

Here, \( \theta_0 \) is the projection of the initial point of the canard on the zeroth order approximations \((\gamma = 0)\) of the slow invariant manifold, i.e. on \( S_{\alpha_0}^{s,1} \), and according to (9), (10) we have \( \eta_0 = \zeta_2'(\theta_0) \).

The equation

\[ \tilde{G}(\theta, \theta_0, 0) = 0 \]

gives a value \( \theta = \theta^* \) which can be calculated numerically. As follows from (19), the value \( \theta^* \) depends on \( \theta_0 \). The fact of this dependence is shown in Figure 7. It should be noted that if we take the initial point close to the origin, we can obtain a high value of the maximal temperature of safe combustion. The closer to the origin, the higher value of the maximal temperature.

Thus, the maximal temperature of safe combustion in the case of an autocatalytic reaction is the maximal temperature \( \theta_{\gamma}^{\max} \) on the canard trajectory starting at the point \((\eta = \eta_0, \theta = 0)\) with \( 0 < \eta_0 < \eta_s \) and

\[ \lim_{\gamma \to 0} \theta_{\gamma}^{\max} = \theta^*(\theta_0). \]

![Figure 7. Dependence of maximal temperature on \( \theta_0 \).](image)

4. Conclusion

The model of combustion of a rarefied gas mixture in an inert medium in the case of an autocatalytic reaction is considered. The connection between the phenomenon of delayed loss of stability in a singularly perturbed differential equation and the estimation of the maximal temperature of safe combustion is stated. It is shown that the maximal temperature of safe combustion is attained during the critical regime separating the domain of explosive chemical reactions and the domain of non-explosive chemical reactions with low temperatures. The critical regime is modelled by the mathematical object called a canard in the modern mathematical literature. Such trajectories pass from the attractive slow invariant manifold to the repulsive one.

The maximal temperature of safe combustion corresponds to the point at which the canard jumps from the repulsive slow invariant manifold. The dependence of maximal temperature on the initial data is obtained.

It should be noted that such an approach was used in [8] to determine the maximal combustion temperature for classic model of autocatalytic combustion.
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