Self-Ignition in Porous Media: Critical Phenomena

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Abstract. The self-ignition of flammable liquid in an inert porous medium is studied. We obtained the complete classification of the possible scenarios of the process using asymptotic and geometrical techniques. This approach allows us to reveal a critical regime which plays a role of a watershed between the safe processes and self-accelerating regimes that lead to the explosion. The realizability conditions for the critical regime are obtained as the explicit asymptotic expression for the control parameter.

1. Introduction

A wide spectrum of thermophysical and chemical processes occurring during combustion, especially in multiphase media, is characterized by a significant difference in time scales (for example, temperature changes vs. concentration changes). Therefore, the singularly perturbed systems of differential equations are used to model combustion processes. For studying such systems different asymptotic methods are usually applied. The asymptotic geometric method used in this paper is based on the theory of integral manifolds (see, for instance, [1, 2] and the references therein). This method allows us to replaces the original system by another system on an integral manifold of lower dimension. The lowering of the dimension occurs due to the decomposition of the original system in the vicinity of the integral surface into the independent “slow” subsystem and the “fast” subsystem. If the slow integral manifold is attractive, then the analysis of the original system can be replaced by the analysis of the slow subsystem retaining a desired degree of accuracy. The use of such approach makes it possible not only to substantially simplify the initial system by reducing its dimension and by eliminating the computational rigidity, but it also gives us a full picture of the dynamics of the physical processes and provides an effective tool for modelling the critical phenomena in these processes. The critical regime corresponds to a chemical reaction separating the domains of self-accelerating reactions and domains of safe reactions. This regime is modelled by a unique trajectory that contains an unstable integral manifold.

This paper deals with the investigation of the critical conditions for self-ignition of combustible fluids in porous insulation materials. This phenomenon is usually caused by a leaking of a combustible liquid into lagging material surrounding a hot pipework. Due to highly insulation environment heat losses are remarkable low and self-ignition may occur as a result of exothermic oxidation reaction. To determine the conditions under which the critical regime is realized, the canard technique [3-6] is used.

We shall study a process which may be defined as the self-ignition in two-phase medium (combustible liquid and inert porous matrix). The possible depletion of oxygen, its diffusion into porous structure, and transport of the liquid or its vapor within the insulation are all ignored. We focus our attention on the
competitive effects of the reactive term of the dispersed liquid and evaporative heat loss. The dimensionless model in this case has the following form [7]:

\[ \dot{u} = Q K_u x e^{-u/a} - (u - u_a) - Q_2 K_2 x e^{-\beta \theta} \], \[ \dot{x} = -K_2 x e^{-\beta \theta} - K_1 x e^{-u/a} \].

(1)

Here, \( u \) is the dimensionless temperature of the reactant phase; the dimensionless concentration \( x \) represents the mass fraction of combustible liquid present in the porous material; the dimensionless parameters \( Q \) and \( K_1 \) characterize the heat of reaction and the reaction frequency, respectively, for the exothermic oxidation reaction, while \( Q_2 \) and \( K_2 \) are the similar terms for the endothermic evaporation reaction; \( \beta \) is the ratio of the enthalpy of vaporization to the activation energy of the oxidation reaction; \( u_a \) is ambient temperature.

Let us introduce the new variables \( \theta \) and \( \tau \) by \( u = \theta + \beta \tau^2 \), \( \tau = \tau \exp(1/\beta) \), \( \beta = u(0) \), and parameters

\[ \varepsilon = \exp \left( -\frac{1}{\beta} \right), a = K_2 \exp \left( \frac{1 - \beta}{\beta} \right), \theta_s = u_a - \beta \tau^2, \mu = \frac{Q_2 K_2}{\beta^2 \tau^2} \exp \left( -\frac{1}{\beta} \right), \nu = \frac{Q_2 K_2}{\beta^2 \tau^2} \exp \left( -\frac{\beta}{\beta} \right). \]

That leads (1) to the system

\[ \dot{\varepsilon} = \mu x \exp \left( \frac{\theta}{1 + \beta \theta} \right) - (\theta - \theta_s) - \nu x \exp \left( \frac{\beta \theta}{1 + \beta \theta} \right) = F(x, \theta), \]

(2)

\[ \dot{x} = -ax \exp \left( \frac{\beta \theta}{1 + \beta \theta} \right) - K_1 x \exp \left( \frac{\theta}{1 + \beta \theta} \right) = G(x, \theta). \]

(3)

which is the singularly perturbed [1] due to the smallness of the parameter \( \varepsilon \) for typical combustible liquids. The chemically relevant phase space \( \Omega \) of system (3), (4) is defined by \( \Omega = \{ x > 0, \theta > -1/\beta \} \).

In [8] the system (1) was investigated numerically under quasi-steady-state assumption that corresponds to the assumption \( \varepsilon = 0 \) for the system (2), (3). This approach allows determining the main types of chemical regimes of the investigated process. The quasi-steady-state assumption is widely used in the theory of combustion and gives good results to draw conclusions about the qualitative behavior of the full system for sufficiently small \( \varepsilon \). However, the critical phenomena are highly sensitive with respect to the parameters. Hence, this fact implies the considerable difficulties under the numerical calculations. Thus, detailed study of this mathematical object is possible with taking into account the small perturbations and use of asymptotic methods, for example, methods of the integral manifolds theory for singularly perturbed systems.

2. Analysis

The trivial solution is the final steady state of the system. The degenerate equation \( F(x, \theta) = 0 \) describes the slow curve \( S \) of (2), (3) [1]. The subset \( S^+(S^-) \) of \( S \) with \( \partial F(x, \theta)/\partial \theta < 0 \) \((> 0)\) is called the stable or attractive (unstable or repulsive) part of \( S \). A point \( A \) on \( S \) in which \( \partial F/\partial \theta = 0 \) is called the jump or turning point. Stable and unstable parts of the slow curve are zeroth order approximations of corresponding stable and unstable slow invariant manifolds. The invariant manifolds lie in an \( \varepsilon \)-neighborhood of the slow curve, except near jump or turning points [1]. The slow curve intersects the axis \( O \theta \) at the point \( \theta = \theta_0 \) and has an asymptote \( \theta = \theta_0 = (\beta_n - 1 - \beta \ln(\mu/\nu))^{-1} \ln(\mu/\nu) \). The shape of the curve \( S \) varies with the relation between values of the parameters, which leads to a change in qualitative behavior of the system. So, if we change the value of one parameter, with fixed values of the other parameters, we can change the type of chemical reaction. Following [8], we consider \( \beta_n \) as a control parameter. For \( \theta_0 = \theta_0 \) we have \( \beta_n = b_0 \), where \( b_0 = 1 + (1 + \beta \theta) \ln(\mu/\nu)/\theta_0 \).
Consider the case $\beta > u_a$ and $b_e < 1$. For $\beta > b_e^+$ the lower branch of $S$ can consist of two stable parts ($s_i^-$) and one unstable part ($s_u^+$), see Figure 1(a). These parts are divided by two turning points, which merge with one another and disappear at a value $\beta_e = b_e^+$ [8], see Figure 1(b). In both cases the trajectories of system (2), (3) move along the stable part of the slow curve to the final steady state. These trajectories correspond to the slow regimes, which are safe, see Figure 2. For $\beta_e > b_e$ the upper and lower branches of $S$ consist of stable ($s_i^-$ and $s_i^+$) and unstable ($s_u^-$ and $s_u^+$) parts, which are divided by the turning points $A_1$ and $A_2$, see Figure 1(d). The system’s trajectories starting at any point of the basin of attraction of $s_i^+$ correspond to the slow regimes.

\[ \beta_e < b_e^+ < b_e; \quad (b) \quad b_e^+ < \beta_e < b_e; \quad (c) \quad \beta_e = b_e; \quad (d) \quad \beta_e > b_e. \]

In the other case, when the initial point is out of the basin of attraction of $s_i^-$, we can observe a thermal explosion (see Figure 3) or a thermal explosion with delay [2, 4]. The thermal explosion with delay occurs when the initial point belongs to the basin of attraction of $s_i^-$ and the system’s trajectories by reaching the jump point $A_1$ along $s_i^-$ at the tempo of the slow variable jump into the explosive regime.

For $\beta_e = b_e$ the point $A_1$ merges with $A_2$ to give one self-intersection point $A$ of the slow curve, see Figure 1(c). As it was noted above, in $\epsilon$-neighborhood of the subset $s_i^-$ ($s_u^+$) there exists a stable (unstable) slow invariant manifold $s_i^-$ ($s_u^+$). For some value $\beta_e = b_e^* = b_e + O(\epsilon)$, ($\epsilon \to 0$), the stable and unstable slow invariant manifolds $s_i^-$ and $s_u^+$ are glued at the point $A$. As a result, for $\beta_e = b_e^*$
system (2), (3) has a canard trajectory [1, 2, 9] which, at first, follows an attractive invariant manifold and then a repulsive one. In both cases the distances are travelled with $O(1)$ as $\varepsilon \to 0$, see Figure 4. This canard simulates the critical regime, separating slow chemical regimes from regimes with a self-acceleration in the case $b_0 < 1$.

![Figure 2](image1.png)

**Figure 2.** (left) The trajectory (the thick line) and the slow curve (the thin line) of (2), (3), and (right) the $x$- and $\theta$-components of the solution in the case of the slow regime: $b = 0.3685$.

![Figure 3](image2.png)

**Figure 3.** The case of the thermal explosion: $b = 1$.

![Figure 4](image3.png)

**Figure 4.** The case of the critical regime: $b = b^* = 0.56827$.

If $\beta > u_\omega$, one can observe the similar transformation of the slow curve (and the qualitative behavior of the system) as shown in Figure 1 but with a decreasing value of the parameter $\beta^*$ ($b^* > b_0$ in this case).

For $b_0 > 1$ plots of the slow curve are mirror images of the graphs shown in Figure 1 with respect to the vertical axis. The thermal behavior of the chemical system is safe for nonsignificant values of the initial concentration of a combustible liquid. Otherwise, the value $\beta^* = b^*$ determines the boundary of the safe region [8].
Our goal is to reveal the sufficient conditions for realization of the critical regime for the case \( b_s < 1 \). As it has been noted above, the main feature is that during the critical regime the temperature attains a high value without explosion. The interest in critical phenomena is occasioned by not only for reasons of safety, but for the fact that in many cases the critical regime is the most effective in technological processes [2-6].

3. Critical phenomena: realizability conditions

Using the method of integral manifolds and the canard techniques [1, 2] it is possible to find the critical value of the parameter \( \beta_c = b^* \) and corresponding trajectory in the form of the asymptotic representations

\[
\theta = \phi(x, \varepsilon) = \phi_0(x) + \varepsilon \phi_1(x) + o(\varepsilon), \quad \beta_c = b^* = b_0 + \varepsilon b_1 + o(\varepsilon). \tag{4}
\]

We write (2), (3) as

\[
\varepsilon \theta^* \left[ a x \exp \left( \frac{\beta_0}{1 + \beta_0} \right) + K_1 x \exp \left( \frac{\theta}{1 + \beta_0} \right) \right] = \theta - \theta^* + \nu x \exp \left( \frac{\beta_0}{1 + \beta_0} \right) - \mu x \exp \left( \frac{\theta}{1 + \beta_0} \right),
\]

or, taking into account (4),

\[
x \left[ (\varepsilon \phi_0^* + \varepsilon^2 \phi_1^*) \right] + \nu x \exp \left( \frac{b_0 \phi_0^*}{1 + \beta_0 \phi_0^*} \right) + a \exp \left( \frac{\phi_0^*}{1 + \beta_0 \phi_0^*} \right) - \mu x \exp \left( \frac{\phi_0^*}{1 + \beta_0 \phi_0^*} \right) = \phi_0^* + \varepsilon \phi_1^* - \theta^* + \nu x \exp \left( \frac{b_0 \phi_0^*}{1 + \beta_0 \phi_0^*} \right) - \mu x \exp \left( \frac{\phi_0^*}{1 + \beta_0 \phi_0^*} \right). \tag{5}
\]

By setting \( \varepsilon = 0 \) in (5) we obtain the slow curve’ equation:

\[
F(x, \phi_0(x)) = \mu x \exp \left( \frac{\phi_0^*}{1 + \beta_0 \phi_0^*} \right) - \phi_0^* + \theta^* - \nu x \exp \left( \frac{b_0 \phi_0^*}{1 + \beta_0 \phi_0^*} \right) = 0. \tag{6}
\]

Conditions for self-intersection of the slow curve in point \( A(x, \phi_0(x)) \)

\[
\partial F(x, \phi_0(x)) / \partial x = \partial F(x, \phi_0(x)) / \partial \phi_0 = 0 \tag{7}
\]

give us the coordinates of the self-intersection point and the zeroth-order approximations for critical value \( b^* \). Indeed, from (6), (7) we obtain

\[
x_a = \frac{(1 + \beta_0 \theta_0^*) \theta_0^*}{\mu \exp \left( \frac{\theta_0^*}{1 + \beta_0 \theta_0^*} \right) \ln (\nu / \mu)}, \quad \phi_0^* (x_a) = \theta_0^*, \tag{8}
\]

\[
b_0 = 1 + (1 + \beta_0 \theta_0^*) \theta_0^* \ln (\mu / \nu). \tag{9}
\]

Equating the coefficients with \( \varepsilon^2 \) in (5) we get

\[
x \phi_0^* \left[ a x \exp \left( \frac{b_0 \phi_0^*}{1 + \beta_0 \phi_0^*} \right) + K_1 x \exp \left( \frac{\phi_0^*}{1 + \beta_0 \phi_0^*} \right) \right] = \phi_0^* + \nu x \exp \left( \frac{b_0 \phi_0^*}{1 + \beta_0 \phi_0^*} \right) - \mu x \exp \left( \frac{\phi_0^*}{1 + \beta_0 \phi_0^*} \right) \tag{10}
\]

From (7) we note that the expression in brackets in the right-hand side of (10) is equal to zero at point \( A \). To avoid a discontinuity in function \( \phi_1(x) \) at \( x_a \), taking into account (8), we put
\[ b_i = \frac{\phi_v'(x_i)(1 + \beta\theta_v)}{v\theta_v} \left[ \frac{K_v \exp \left( \frac{(1 - b_v)\theta_v}{1 + \beta\theta_v} \right) + a}{\theta_v} \right]. \]

or, taking into account (6) and (7),

\[ b_i = \frac{2\mu^s}{\theta_v} \left( 1 + \beta\theta_v \right)^{\mu^s} \ln \frac{v}{\mu} \exp \left( \frac{3\theta_v}{1 + \beta\theta_v} \right) \left[ \frac{K_v}{\mu} + a \right] \left[ 2\beta \left( 1 + \beta\theta_v \right) - 2 + \frac{(1 + \beta\theta_v)}{\theta_v} \ln \frac{v}{\mu} \right]. \]  

Thus, the expressions (6), (9)–(11) determine the first-order approximation for the canard and the corresponding critical value \( \beta^* = \beta^* \). It should be noted that it is not possible to explicitly solve equation (6) with respect to \( \phi_v \), while the critical value \( b^* \) has been found in the explicit form. However, one can use the implicit or parametric representation for slow invariant manifold [1] to obtain an approximation of the canard.

4. Conclusion

In this paper the model of self-ignition of combustible fluids in an inert porous medium has been studied. The realizability conditions for the critical regime have been obtained as the explicit asymptotic expression for the control parameter. It was shown that the critical regime is modelled by the canard. This regime plays the role of a watershed between the safe processes and regimes with self-acceleration that leads to an explosion. It should be noted that the critical regime is not a slow regime, since the temperature may attain a high value, nor an explosive regime, as the temperature increases at the tempo of the slow variable. Thus, for the examined model the new type of the safe regime has been revealed.

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