Repulsive Invariant Manifolds in Modeling the Critical Phenomena

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Abstract The paper shows how the repulsive invariant manifolds of multiscale dynamical systems are used for modeling the critical phenomena. A dynamical model of fuel spray ignition is considered to illustrate this approach.

1 Introduction

The paper outlines an approach to modeling the critical phenomena in multiscale dynamical models. Such models are usually described by singularly perturbed systems of differential equations to reflect the significant distinction in characteristic relaxation times of different processes. The approach is based on the geometric asymptotic method of invariant manifolds; see [4].

By a critical phenomenon, we mean a sharp change in a model's dynamics via a transition from a slow process to a self-accelerating mode. According to the theory of invariant manifolds, processes with self-acceleration correspond to trajectories that either has no common point with an attractive slow invariant manifold, or leave it after a while; see [3]. The last situation occurs when the trajectory reaches a boundary separating the attractive slow invariant manifold from repulsive one.

Using a fuel spray ignition model, we demonstrate how the repulsive slow invariant manifold can be used for modeling the critical phenomena.

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2 Model

The model of ignition and combustion of a fuel spray is formulated using an adiabatic approach. The fuel spray is considered as a two-phase medium: the combustible gas mixture and the combustible liquid droplets. The effects of changes in pressure are neglected. The usual assumption is made that the thermal conductivity of the liquid phase is much greater than that in the gas phase. Thus, the heat transfer coefficient in the liquid gas mixture is supposed to be defined by the thermal properties of the gas phase. The droplets boundary is assumed to be on a saturation line, i.e., the liquid temperature is constant and is equal to the liquid saturation temperature. The combustion reaction is modeled as a first order, highly exothermic chemical reaction. The model is built with the usual assumptions of the theory of combustion processes in chemical homogeneity at each point of the reaction vessel. The dimensionless model has the following form (see [1])

$$\gamma \frac{d\theta}{d\tau} = \eta \exp\left(\frac{\theta}{1+\beta\theta}\right) - \varepsilon_1 r\theta(1+\beta\theta), \tag{1}$$

$$\frac{dr^3}{d\tau} = -\varepsilon_1\varepsilon_2 r\theta, \tag{2}$$

$$\frac{d\eta}{d\tau} = -\eta\frac{1}{1+\beta\theta}\exp\left(\frac{\theta}{1+\beta\theta}\right) + \varepsilon_1 r\psi\theta, \tag{3}$$

where θ is the dimensionless fuel gas temperature; r is the dimensionless radius of the droplets; η is the dimensionless concentration of the flammable gas; τ is the dimensionless time; γ is the dimensionless parameter equal to the final dimensionless adiabatic temperature thermally isolated system after the explosion; β gives the initial temperature; ε_1, ε_2 characterize the interaction between the gas and liquid phases; ψ is a parameter characterizing the ratio of the energy of combustion gas mixture to the liquid evaporation energy.

The initial conditions for the Eqs. (1)–(3) are

$$\theta(0) = 0, \quad \eta(0) = 1, \quad r(0) = 1.$$

Appropriate combination of Eqs. (1)–(3) and integration over time yields the following energy integral

$$\eta - 1 + \frac{\gamma}{\beta}\ln(1+\beta\theta) + \frac{\psi-1}{\varepsilon_2}\left(r^3-1\right) = 0,$$

which allows to reduce the order of the system (1)–(3) to the form

$$\gamma \frac{d\theta}{d\tau} = \left(1 - \frac{\gamma}{\beta}\ln(1+\beta\theta) - \frac{\psi - 1}{\varepsilon_2}\left(r^3 - 1\right)\right)\exp\left(\frac{\theta}{1+\beta\theta}\right) - \varepsilon_1 r\theta(1+\beta\theta), \tag{4}$$

$$\frac{dr^3}{d\tau} = -\varepsilon_1\varepsilon_2 r\theta. \tag{5}$$

The degenerate equation, which follows from the fast subsystem (4) for $\gamma = 0$, describes a slow curve

$$\Lambda(\theta, r) = \left(1 - \frac{\gamma}{\beta}\ln(1+\beta\theta) - \frac{\psi - 1}{\varepsilon_2}\left(r^3 - 1\right)\right)\exp\left(\frac{\theta}{1+\beta\theta}\right) - \varepsilon_1 r\theta(1+\beta\theta) = 0$$

in the phase plane. The flow of system (4), (5) near the slow curve has a velocity of $O(1)$ as $\gamma \to 0$, while far from the slow curve the variable θ is changed very rapidly. In a γ neighborhood of the slow curve, there exists a slow invariant manifold of the system which is defined as an invariant surface of slow motions.

The set of points on the slow curve where $\partial\Lambda/\partial\theta < 0$ ($\partial\Lambda/\partial\theta > 0$) forms a stable (unstable) part of the slow curve. The stable and unstable parts of the slow curve are the zero-order approximations ($\gamma = 0$) of the stable (or attractive) and unstable (or repulsive) slow invariant manifolds of the system (4), (5), respectively.

For $0 < \psi < 1 - \varepsilon_2$, the slow curve is concave, see Fig. 1a. The part PT of the slow curve is stable while the part TQ is unstable. The ordinate of the point T depending on the parameters' values can be equal to, greater, or less than 1. If the point T has an ordinate greater than 1, a trajectory of the system starts from the initial point and tends to the stable part PT of the slow curve. Then it follows PT to the origin. This is the case of a slow combustion regime; see the trajectory $C''JP$ in Fig. 1a.

If the point T has an ordinate less than 1, then a trajectory of the system will pass beyond the basin of attraction of the PT. This case corresponds to an explosion regime; see the trajectory $C'D$ in Fig. 1a.

3 Critical Phenomenon

A critical phenomenon corresponds to the case when the trajectory of the system falls into a small vicinity of the point T and passes along the unstable part TQ of the slow curve (see the trajectory CTQ in Fig. 1a). This trajectory corresponds to the critical regime, which separates the safe regimes from explosive modes [3, 5].

The crucial result is that the repulsive slow manifold may be used to construct the critical trajectory CTQ and to calculate the corresponding value of a control parameter of the system, say, ε_1. To do this, we use the asymptotics proposed in [2]. To make this use eligible, we introduce the new "reverse" time $t = -\tau$ in (4), (5) that make the slow invariant manifold near TQ attractive; see [3].

The part CT of the critical trajectory can be represented in the form

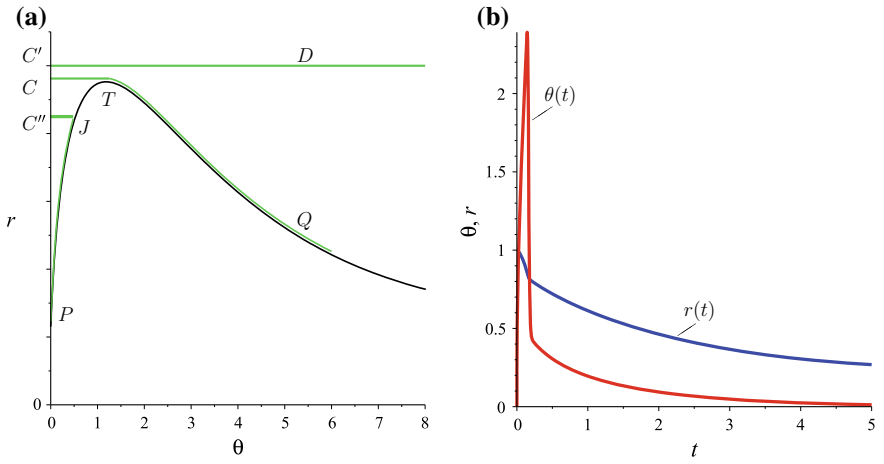

Fig. 1 **a** The slow curve (black) and the trajectories (green) of the system (4), (5) with $0 < \psi < 1 - \varepsilon_2$ in the limit case ($\gamma = 0$); **b** the solutions of (1)–(3) in the case of critical regime for $\gamma = 0.01$, $\varepsilon_1 = 2.2100108$, $\varepsilon_2 = 0.8$, $\beta = 0.05$, $\psi = 0.19$

$$r(\theta, \gamma) = r^* + \gamma^{\frac{2}{3}} \Gamma_0^{\frac{2}{3}} \Omega \operatorname{sign} f(\theta^*, r^*) + \frac{1}{3}\gamma \ln \frac{1}{\gamma} \Gamma_1 \operatorname{sign} f(\theta^*, r^*) + O(\gamma), \quad (6)$$

where θ^*, r^*, denote the coordinates of the point T, the functions f and g are the right parts of the system (4), (5) after the transition to the reverse time t,

$$\Omega = 2.338107, \quad \Gamma_0 = \sqrt{\frac{2}{|g_{\theta\theta}(\theta^*, r^*) g_r(\theta^*, r^*)|}}\, |f(\theta^*, r^*)|,$$

$$\Gamma_1 = \frac{6 g_{\theta\theta}(\theta^*, r^*) f_\theta(\theta^*, r^*) - 2 g_{\theta\theta\theta}(\theta^*, r^*) f(\theta^*, r^*)}{3 g_{\theta\theta}^2(\theta^*, r^*)}.$$

The coordinates θ^*, r^* can be found from the system $g(\theta^*, r^*) = g_\theta(\theta^*, r^*) = 0$. Substituting all the found values into (6) and setting $r = 1$ since the point C has the coordinate $r = 1$, we obtain the equation for calculation the critical parameter value $\varepsilon_1 = \varepsilon_1^*$ in the form

$$\varepsilon_1^* = \varepsilon_{10} + \gamma^{\frac{2}{3}} \varepsilon_{11} + \gamma \ln \frac{1}{\gamma} \varepsilon_{12} + O(\gamma).$$

A direct calculation gives

$$\varepsilon_{10} = \frac{pe(\psi - 1)}{\varepsilon_2}, \quad \varepsilon_{11} = -54\Omega(\psi - 1)^3 \sqrt[3]{\frac{2}{9}} \mu_1^{\frac{4}{3}} \mu_{23}^{-\frac{2}{3}} \varepsilon_{10}^{-\frac{4}{3}} \varepsilon_2^{-\frac{4}{3}}$$

$$\times \left\{(1-6\beta)\left[\frac{\psi-1}{\varepsilon_2}(\mu_{23}^3-1)-1\right]e+2\varepsilon_{10}\mu_{23}\beta\right\}^{-\frac{1}{3}}\left[3\mu_{23}^2 e\frac{\psi-1}{\varepsilon_2}+\varepsilon_{10}(1+\beta)\right]^{-\frac{1}{3}},$$

$$\varepsilon_{12}=\frac{\varepsilon_{10}\varepsilon_2}{3\mu_{23}}\left\{(1-14\beta)\left[\frac{\psi-1}{\varepsilon_2}(\mu_{23}^3-1)-1\right]e+4\varepsilon_{10}\mu_{23}\beta\right\}$$

$$\times\left\{(1-6\beta)\left[\frac{\psi-1}{\varepsilon_2}(\mu_{23}^3-1)-1\right]e+2\varepsilon_{10}\mu_{23}\beta\right\}^{-2},$$

where

$$q=\frac{\varepsilon_2+\psi-1}{\psi-1},\mu_1=\sqrt{\frac{q^2}{4}+\frac{\varepsilon_{10}^3\varepsilon_2^3}{27(\psi-1)^3}},\mu_2=\sqrt[3]{\frac{q}{2}+\mu_1},\mu_3=\sqrt[3]{\frac{q}{2}-\mu_1},\mu_{23}=\mu_2+\mu_3,$$

and p is a root of the equation

$$1=\sqrt[3]{\frac{q}{2}+\sqrt{\frac{q^2}{4}+\frac{p^3}{27}}}+\sqrt[3]{\frac{q}{2}-\sqrt{\frac{q^2}{4}+\frac{p^3}{27}}}.$$

It should underline that the main feature of the critical regime is that during it the temperature of the combustible mixture can reach a high value within the framework of a safe process, see Fig. 1b.

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