Analysis of the threshold phenomena in a dynamic model of a fuel spray ignition

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Abstract. Computer simulation of the dynamics of a fuel spray ignition revealed the presence of threshold phenomena. A threshold phenomenon means as a sharp change in the dynamics of the process. A geometric approach based on the theory of integral manifolds is used to model and analyze threshold phenomena in a dynamic model of ignition and burning of a fuel spray.

1. Introduction

In this paper, a dynamic model of the ignition and combustion of a fuel spray is investigated. The main dynamic features of sprays combustion are determined by the heat loss due to the evaporation of a combustible liquid medium, i.e. droplets, and heat release during an exothermic oxidation reaction in the gas phase. The competition between these processes determines whether the reaction will be safe or will proceed into self-accelerating mode that can lead to the explosion. In this paper the main attention is paid to the analysis of the threshold phenomena, which are considered as the boundary of the process’ safety.

2. Spray ignition model

The model of the ignition and combustion of a fuel spray is suggested using an adiabatic approach [1-3]. The fuel spray is considered as a two-phase medium: combustible gas mixture — combustible liquid droplets. The pressure change in the reaction volume and its effect on the combustion process is assumed a slight and is omitted. The usual assumption is made that the thermal conductivity of the liquid phase is much greater than that in the gas phase [4-19]. Thus, the heat transfer coefficient in the liquid gas mixture is supposed to be defined by the thermal properties of the gas phase. The drop 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 and in the dimensionless form has the form [20]:

\[ \gamma \frac{d\theta}{d\tau} = \eta \exp \left( \frac{\theta}{1+\beta \theta} \right) - \epsilon_1 r \theta (1+\beta \theta), \quad (1) \]

\[ \frac{dr}{d\tau} = -\epsilon_1 \epsilon_2 r \theta, \quad (2) \]

\[ \frac{d\eta}{d\tau} = -\eta \frac{1}{1+\beta \theta} \exp \left( \frac{\theta}{1+\beta \theta} \right) + \epsilon_1 \psi r \theta, \quad (3) \]
where $\theta$ is the dimensionless fuel gas temperature; $r$ is the dimensionless radius of the drops; $\eta$ is the dimensionless concentration of flammable gas; $\tau$ is the dimensionless time; $\gamma$ is the dimensionless parameter equal to the final dimensionless adiabatic temperature thermally isolated system after the explosion; $\beta$ gives the initial temperature; $\epsilon_1, \epsilon_2$ characterize the interaction between the gas and liquid phases; $\psi$ is a parameter characterizing the ratio of the energy of combustion gas mixture to the liquid evaporation energy.

The initial conditions for the equations (1)-(3) are:

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

Appropriate combination of equations (1)-(3) and integration over time yields the following energy integral

$$\eta - 1 + \frac{\gamma}{\beta} \ln(1 + \beta \theta) + \frac{\psi - 1}{\epsilon_2} (r^3 - 1) = 0,$$

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

$$\gamma \frac{d\theta}{d\tau} = \left( 1 - \frac{\gamma}{\beta} \ln(1 + \beta \theta) - \frac{\psi - 1}{\epsilon_2} (r^3 - 1) \right) \times \exp \left( \frac{\theta}{1 + \beta \theta} \right) - \epsilon_1 r \theta (1 + \beta \theta),$$  

$$\frac{dr}{d\tau} = -\epsilon_1 \epsilon_2 \theta r.$$  

Thus, the dynamic of the system depends on five dimensionless parameters: $\beta \ll 1, \gamma \ll 1, \epsilon_1, \epsilon_2, \psi$.

In [21], using the geometric approach based on the theory of integral manifolds for singularly perturbed systems [22-27], the existence of three types of reaction modes was established. Such regimes are the safe slow combustion regime, the thermal explosion, and the critical regime playing a role of the boundary between these two first modes. Recall the main results of this work.

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

$$\Lambda(\theta, r) = \left( 1 - \frac{\gamma}{\beta} \ln(1 + \beta \theta) + \frac{(\psi - 1)(1 - r^3)}{\epsilon_2} \right) \exp \left( \frac{\theta}{1 + \beta \theta} \right) - \epsilon_1 r \theta (1 + \beta \theta) = 0$$

in the phase plane. The flow of the system (4), (5) near the slow curve has a velocity of order of one as $\gamma \to 0$ while far from the slow curve the variable $\theta$ is changed very fast. In $\gamma -$ 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 at which $\partial \Lambda / \partial \theta < 0$ ($\partial \Lambda / \partial \theta > 0$) forms the 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 $0 < \psi < 1 - \epsilon_2$ the slow curve has the shape similar to that shown in Figure 1. 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 1 or be greater (or less) than 1. If the point $T$ has an ordinate greater than 1 then a trajectory of the system starting from the initial point tends to stable part $PT$ of the slow curve and follows it to the origin. This is the case of the slow combustion regime; see the trajectory $CTP$ in Figure 1.

If the point $T$ has an ordinate less than 1 then a trajectory of the system starting from the initial point will pass beyond the basin of attraction of the stable part of the slow curve. This is the case of the explosion regime; see the trajectory $CD$ in Figure 1.

Figures 2, 3 summarized results of a numerical study of system (4), (5) for the slow combustion regime for $\gamma = 0.01, \epsilon_1 = 3.5, \epsilon_2 = 0.8, \beta = 0.05, \psi = 0.19$. 


3

Figure 1. Slow curve (black) and the trajectories (green) of the system (4), (5) with $0 < \psi < 1 - \varepsilon_2$ in limit case ($\gamma = 0$).

Figure 2. Trajectory of the system (4), (5) in the case of the slow combustion regime.

Figure 3. The solutions of the system (1)-(3) vs $t$ in the case of the slow combustion regime.

Figures 4, 5 depict the trajectory of the system (4), (5) and the solutions of the system (1)-(3) in the case of thermal explosion for $\varepsilon_1 = 2.0$, other parameters values are the same as for figures 2 and 3. In this case the temperature $\theta$ increases rapidly and achieves a high value (Figure 4) while the other phase variables are subject to minor changes (Figure 5).

The critical regime 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 Figure 1. The critical regime separates the explosive regimes from the safe combustion modes [28, 29]. The crucial result is that the unstable slow manifold may be used to construct the critical trajectory $CTQ$ and to calculate the corresponding value of a control parameter, say, $\varepsilon_1$, of the system.

For this goal we use the asymptotics proposed in [30].

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

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

where $r^*, \theta^*$ denote the coordinates of the point $T$,

$$\omega = 2.338107, f(\theta, r) = \varepsilon_1 \varepsilon_2 r \theta,$$

$$g(\theta, r) = \left(-1 + \frac{\gamma}{\beta} \ln(1 + \theta \beta) + \frac{\psi - 1}{\varepsilon_2}(r^3 - 1)\right) \exp\left(\frac{\theta}{1 + \beta \theta}\right) + \varepsilon_1 r \theta (1 + \theta \beta),$$
The functions $f$ and $g$ in the representation (6) are the right parts of the system (4), (5) after the transition to the inverse time that make the part $TQ$ of the slow curve stable.

The coordinates $r^*, \theta^*$ can be calculated from the system [23] $g(r^*, \theta^*)=g_0(r^*, \theta^*) = 0$, i.e.,

$$
\left(-1 + \frac{\psi}{\beta} \ln(1 + \beta \theta^*) + \frac{\psi - 1}{\epsilon_2} (r^{*3} - 1) \right) \exp \left( \frac{\theta^*}{1 + \beta \theta^*} \right) + \epsilon_1 r^* \theta^* (1 + \beta \theta^*) = 0,
$$

$$
\frac{\gamma}{\beta (1 + \beta \theta^*)} \exp \left( \frac{\theta^*}{1 + \beta \theta^*} \right) + \frac{1}{(1 + \beta \theta^*)^2} \times \left(-1 + \frac{\gamma}{\beta} \ln(1 + \beta \theta^*) + \frac{\psi - 1}{\epsilon_2} (r^{*3} - 1) \right)
$$

$$
\times \exp \left( \frac{\theta^*}{1 + \beta \theta^*} \right) + \epsilon_1 r^* (1 + \beta \theta^*) + \epsilon_1 r^* \theta^* \beta = 0.
$$

Due to the smallness of the parameter $\beta$, the coordinates $r^*, \theta^*$ can be found in the form $r^* = r_0 + r_1 \beta + O(\beta^2), \quad \theta^* = \theta_0 + \theta_1 \beta + O(\beta^2)$, where

$$
r_0 = \sqrt{\frac{q}{2} + \frac{q^2}{4} + \frac{p^3}{27}}, \quad \theta_0 = 1, \quad \theta_1 = 3.
$$

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 of the critical values of the parameter $\epsilon_1 = \epsilon_1^*$ in the form of asymptotic representation

$$
\epsilon_1^* = \epsilon_{10} + \gamma^2 \epsilon_{11} + \gamma \ln \frac{1}{\gamma} \epsilon_{12} + O(\gamma).
$$

The direct calculation gives...
\[ \varepsilon_{10} = \frac{\bar{p}(\psi - 1)}{\varepsilon_2}, \]

\[ \varepsilon_{11} = \frac{3}{\varepsilon_2} \frac{2}{\sqrt{\Omega 6(\psi - 1)^3 \varepsilon_2^2}} \frac{(\varepsilon_{10} \varepsilon_2)^3}{q^2} \frac{q^2}{27(\psi - 1)^3} - \frac{1}{3} \]

\[ \times \psi - 1 \left( \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} - 1 \right) \]

\[ \times e(\psi - 1)^3 \left( \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \varepsilon_{10} \right) \]

\[ \times \left( \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \frac{1}{3} \sqrt{\varepsilon_{10}} \right) \]

\[ \times \left( 4q + 12 \frac{q^2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + 6 \frac{q}{\sqrt{2(\psi - 1)^3}} - 1 \right), \]

where \( \bar{p} \) is a root of the equation

\[ 1 = \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \frac{3}{\varepsilon_2} \frac{2}{\sqrt{4 + \frac{27(\psi - 1)^3}{q^2}}} + \frac{\bar{p}^3}{27}. \]

The value \( \varepsilon_1 = \varepsilon_1^* \), at which the trajectory of (4), (5) contains the unstable manifold is said to be critical, i.e. this regime is not a slow combustion regime, since the temperature achieves a high value, and is not explosive, as the temperature increases at the tempo of the slow variable as this is the slow manifold. The value of \( \varepsilon_1 = \varepsilon_1^* \), gives the critical trajectory which separates the explosion modes (\( \varepsilon_1 < \varepsilon_1^* \)) from the slow regimes (\( \varepsilon_1 > \varepsilon_1^* \)) which are characterized by a slowdown of the reaction with small degrees of conversion and heating up is limited from above by \( \theta < \theta^* \) at \( T \).

Figures 6, 7 show the trajectory of the system (4), (5) and the solutions of the system (1)-(3) in the case of critical regime for \( \varepsilon_1 = 2.2100108 \), other parameters values are the same as for figures 2 and 3.

3. Conclusion
The dynamic model of a fuel spray ignition was studied by the methods of the geometric theory of singular perturbations. The realizability conditions for the critical regime was obtained in the form of the asymptotic expression for the control parameter. 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. It was shown that the critical regime plays the role of a watershed between the slow combustion regimes and the thermal explosion.

**Figure 6.** Trajectory of the system (4), (5) in the case of critical regime.

**Figure 7.** The solutions of the system (1)-(3) in the case of critical regime.

The analytical calculations presented in this paper are of utmost importance for the realization of safe high-temperature processes.

### 4. References

[1] Stone R 1992 *Introduction to Internal Combustion Engines* (The MacMillan Press Ltd, Second Edition)

[2] Sazhin S S, Shchepakina E and Sobolev V 2010 *Mathematical and Computer Modelling* **52**(3-4) 529

[3] Sazhin S S, Feng G, Heikal M R, Goldfarb I, Goldshtein V and Kuzmenko G 2001 *Combustion and Flame* **124**(4) 684

[4] Healy D P and Young J B 2005 *Proc. Royal Soc. London, Ser. A* **461** 2197

[5] Kaplanski F B and Rudi Y A 2005 *Phys. Fluids* **17**(8) 087101 DOI: 10.1063/1.1996928

[6] Zubkov V S, Cossali G E, Tonini S, Rybdylova O, Crua C, Heikal M and Sazhin S S 2017 *International Journal of Heat and Mass Transfer* **108** 2181

[7] Tonini S and Cossali, G 2013 *International Journal of Heat and Mass Transfer* **60** 236

[8] Rybdylova O, Osiptsov A N, Sazhin S S, Begg S and Heikal M 2016 *International J of Heat and Fluid Flow* **58** 93

[9] Sazhin S 2014 *Droplets and Sprays* (London: Springer)

[10] Sazhina E M, Sazhin S S, Heikal M R, Babushok V I and Johns R 2000 *Combustion Science and Technology* **160** 317

[11] Lebedeva N A, Osiptsov A N and Sazhin S S 2013 *Atomization and Sprays* **23**(1) 47

[12] Crua C, Heikal, M R and Gold and M R 2015 *Fuel* **157** 140

[13] Sazhin S S 2017 *Fuel* **196** 69

[14] Rybdylova O and Sazhin S S 2017 *Journal of Physics: Conference Series* **811** 012014 DOI:10.1088/1742-6596/811/1/012014

[15] Zaripov T S, Gifianov A K, Begg S M, Rybdylova O, Sazhin S S and Heikal M R 2017 *Atomization and Sprays* **27**(6) 493

[16] Rybdylova O, Sazhin S S, Osiptsov A N, Kaplanski F B, Begg S and Heikal M 2018 *Applied Mathematics and Computation* **326** 159

[17] Papoutsakis A, Rybdylova O D, Zaripov T S, Danaila, L, Osiptsov A N and Sazhin S S 2018 *International Journal of Multiphase Flow* **104** 233

[18] Sazhin S S, Rybdylova O, Pannala A S, Somavarapu S and Zaripov S K 2018 *International Journal of Heat and Mass Transfer* **122** 451
[19] Basu S, Agarwal A K, Mukhopadhyay A and C Patel C (Editors) 2018 Droplet and Spray. Application for Combustion and Propulsion (Singapore: Springer)

[20] Goldfarb I, Gol’dshtein V, Shreiber I and Zinoviev A 1996 Proceedings of the 26th Symposium on Combustion (Pittsburgh: The Combustion Institute) 1557

[21] Agataeva A Zh and Shchepakina E A 2016 CEUR Workshop Proceedings 1638 484

[22] Sobolev V A and Shchepakina E A 1993 Combustion, Explosion, and Shock Waves 29(3) 378

[23] Shchepakina E, Sobolev V and Mortell M P 2014 Singular Perturbations. Introduction to System Order Reduction Methods with Applications In: Lecture Notes in Mathematics vol. 2114 (Berlin-Heidelberg-London: Springer)

[24] Gorelov G N, Shchepakina E A and Sobolev V A 2006 Journal of Engineering Mathematics 56(2) 143

[25] Gavin C, Pokrovskii A, Prentice M and Sobolev V 2006 Journal of Physics: Conference Series 55 80

[25] Pokrovskii A, Shchepakina E and Sobolev V 2008 Journal of Physics: Conference Series 138 012019

[27] Pokrovskii A, Rachinskii D, Sobolev V and Zhezherun A 2011 Applicable Analysis 90(7) 1123

[28] Shchepakina E and Korotkova O 2011 JOSA B: Optical Physics 28(8) 1988

[29] Shchepakina E and Korotkova O 2013 Discrete and Continuous Dynamical Systems - Series B 18(2) 495

[30] Mishchenko E F and Rozov N Kh 1980 Differential Equations with Small Parameters and Relaxation Oscillations (New York: Plenum Press)

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