STOCHASTIC GENERATION OF OSCILLATIONS IN THE 3D-MODEL OF COOL-FLAME COMBUSTION OF A HYDROCARBON MIXTURE

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Abstract

The stochastic model of cool-flame combustion of a hydrocarbon mixture is considered. For this 3D model, noise excitement of large-amplitude oscillations in the parametric zone, where the deterministic model has a single equilibrium attractor, is studied. By statistics of interspike intervals, a phenomenon of anti-coherence resonance is revealed. To estimate threshold intensities of noise that causes excitement, stochastic sensitivity technique and method of principal directions are applied.

Key words

combustion, mathematical model, random disturbances, excitement, method of principal directions

1 Introduction

At present, mathematical modelling of thermochemical kinetics is actively used to study complex combustion processes [Williams, 2018; Bykov et al., 2018]. Even in the class of two-dimensional dynamic models, a wide diversity of oscillatory regimes was found (see, e.g. [Uppal et al., 1974; Sheplev et al., 1998]). In these studies, researchers rely on the mathematical theory of bifurcations and computer simulations.

Mathematically, an appearance of oscillatory regimes is usually associated with the existence of limit cycles. In the studies [Bykov et al., 1980; Bykov et al., 2018], such a connection was used to explain the mechanisms that generate oscillatory forms of kinetics in three-dimensional combustion models.

Recently, the study of stochastic models that take into account the inevitable random perturbations has attracted considerable interest of researchers. Indeed, the combination of strong nonlinearity and stochasticity can generate new unexpected modes of dynamics that have no analogues in the original deterministic models [Horsthemke and Lefever, 1984; Anishchenko et al., 2007; Lindner et al., 2004; Bashkirtseva, 2016; Kremer, 2021; Romero-Meléndez and Castillo-Fernández, 2022]. A constructive role of noise in two-dimensional models of thermochemical kinetics was revealed and investigated (see, e.g. [Lemarchand and Nowakowski, 2005; Ryashko, 2021]). Stochastic effects in the three-dimensional combustion model in a zone of limit cycles was studied in [Bashkirtseva and Slepukhina, 2022].

This paper aims to show how oscillatory regimes can be induced by noise in a zone where the stable equilibrium is a single attractor of the deterministic model. In our study, we use the three-dimensional model of the cool-flame combustion of an n-heptane-isooctane mixture [Bykov et al., 1980].

In Section 2, we briefly present results of bifurcation analysis of the deterministic model. In Section 3, we study an impact of noise in the parameter zone where this deterministic model possesses the only equilibrium attractor. Here, noise-induced excitement of oscillations of large amplitudes is studied by statistics of interspike intervals. A phenomenon of anti-coherence resonance is discussed. To estimate threshold intensities of noise that causes excitement, the stochastic sensitivity technique [Bashkirtseva and Ryashko, 2018; Ryashko, 2018;

Alexandrov et al., 2021] and the method of principal directions are applied.

2 Deterministic model

Consider the three-dimensional model which describes the cool-flame combustion of a mixture of two hydrocarbons (n-heptane and isooctane) [Bykov et al., 1980]:

$$\begin{aligned} \dot{x}_1 &= f_1(y)\,(1-x_1) - x_1 \\ \dot{x}_2 &= f_2(y)\,(1-x_2) - x_2 \\ \dot{y} &= \beta_1\, f_1(y)\,(1-x_1) + \beta_2\, f_2(y)\,(1-x_2) + \\ &\quad +(1-y) - s\,(y-\bar{y}), \end{aligned} \tag{1}$$

where

$$f_i(y) = Da_i \,\exp\left[\gamma_i \left(1 - \frac{1}{y}\right)\right], \quad i = 1, 2.$$

Here, x_1 and x_2 are the concentrations of two reagents, and y is the temperature. Da_i, β_i, γ_i, s, $\bar{y}$ are dimensionless parameters of the model. In this article, we fix the parameters as in [Bykov et al., 2018],

$$Da_1 = 0.14,\; Da_2 = 0.001,\; \beta_1 = 0.25,\; \beta_2 = 0.5,$$
$$s = 2,\; \bar{y} = 1, \gamma_2 = 40,$$

and study the behavior of the system when γ_1 is varied. Fig. 1 shows the bifurcation diagram of the system (1) in

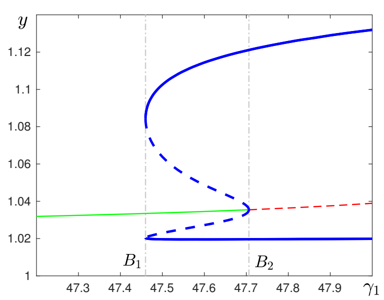

Figure 1. Bifurcation diagram of the deterministic system (1): y-coordinates of stable (greed solid) and unstable (red dashed) equilibria; minimal and maximal values of y-coordinate along stable (blue solid) and unstable (blue dashed) limit cycles, in dependence on the parameter γ_1.

the region $\gamma_1 \in (47.2, 48)$. For $\gamma_1 < B_2 \approx 47.71$, there is a unique stable equilibrium, which loses its stability at $\gamma_1 = B_2$ due to the subcritical Andronov-Hopf bifurcation, when an unstable limit cycle is born. As a result of the saddle-node bifurcation of limit cycles, a stable limit cycle appears in the system at $\gamma_1 = B_1 \approx 47.46$. Thus, in the region $B_1 < \gamma_1 < B_2$, the stable limit cycle coexists with the stable equilibrium, and for $\gamma_1 > B_2$, the only attractor of the system is the stable limit cycle.

In this paper, we focus on the zone $\gamma_1 < B_2$, where the system (1) is in the monostable equilibrium regime. Fig. 2 shows an example of a phase portrait in this region. Here, the system is excitable: a small deviation from the stable equilibrium can result in trajectories of large amplitudes.

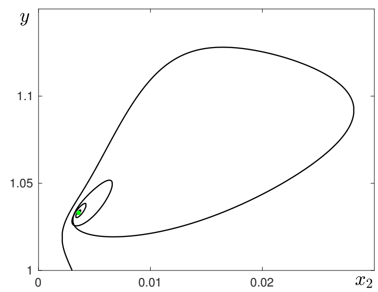

Figure 2. Phase portrait for $\gamma_1 = 47.4$: projection of a phase trajectory (solid) and the stable equilibrium (circle) on the plane $x_2 - y$.

3 Stochastic generation of large-amplitude oscillations

Let us study effects of noise on the system (1) in the equilibrium mode. For this, consider the stochastic model

$$\begin{aligned} \dot{x}_1 &= f_1(y)\,(1-x_1) - x_1 \\ \dot{x}_2 &= f_2(y)\,(1-x_2) - x_2 \\ \dot{y} &= \beta_1\, f_1(y)\,(1-x_1) + \beta_2\, f_2(y)\,(1-x_2) + \\ &\quad +(1-y) - s\,(y-\bar{y}) + \varepsilon\xi(t), \end{aligned} \tag{2}$$

where $\xi(t)$ is the standard white Gaussian noise with the properties $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\xi(t+\tau) \rangle = \delta(\tau)$ and the intensity ε.

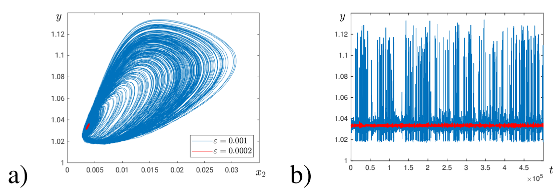

Figure 3. Projections of system (2) random trajectories on the $x_2 - y$-plane (a) and corresponding time series $y(t)$ (b) starting from the stable equilibrium for $\gamma_1 = 47.45$ for $\varepsilon = 0.0002$ (red) and $\varepsilon = 0.001$ (blue).

Fig. 3 shows random trajectories of the system (2) starting at the stable equilibrium and the corresponding time series $y(t)$ for different values of the noise intensity ε. One can see that for $\varepsilon = 0.0002$, the trajectory stays close to the deterministic equilibrium, while for $\varepsilon = 0.001$, large-amplitude oscillations far away from the equilibrium appear.

Such generation of large-amplitude oscillations by noise is observed also for other values of the parameter γ_1. Fig. 4 displays y-coordinates of random states in dependence on γ_1, for several fixed values of ε. One can notice that with an increase of the noise intensity, the zone of large-amplitude oscillations expands, so that they appear for smaller values of γ_1. This can be considered as a stochastic shift of the bifurcation point.

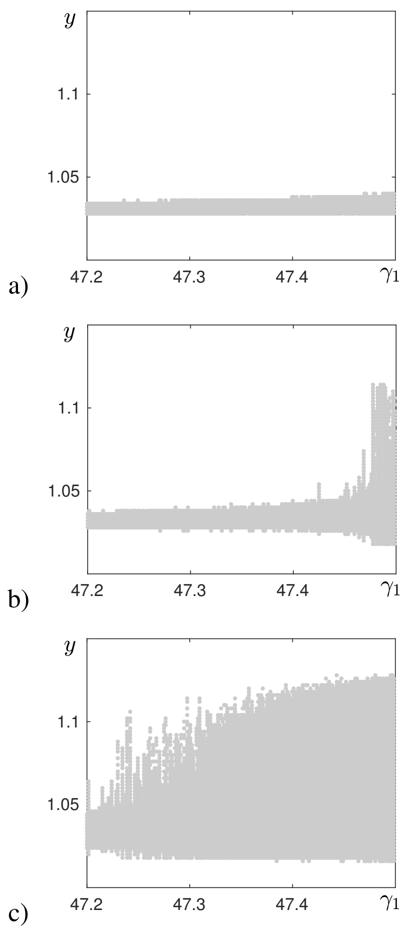

Figure 4. Distribution of y-coordinates of system (2) random states in dependence on γ_1 for several fixed values of noise: a) $\varepsilon = 0.0002$, b) $\varepsilon = 0.0003$, c) $\varepsilon = 0.0005$.

The transition to large-amplitude oscillations from the equilibrium mode can be also traced analyzing interspike intervals statistics. Interspike intervals are commonly referred to as time intervals between two consecutive peaks of large amplitude in oscillations. In Fig. 5, mean values m and coefficients of variation CV for such intervals are plotted. For weak noise, the values m are large, since stochastic trajectories are the most likely to locate near the deterministic equilibrium and large-amplitude spikes appear extremely rare. As the intensity ε increases and becomes larger than some threshold, the values m abruptly decrease, which indicates the onset of stochastic generation of large-amplitude oscillations. For the same levels of noise, the coefficients of variation change from zero to sufficiently large values, which marks a large variation in lengths of interspike intervals in forming oscillations. This effect is known as anti-coherence resonance.

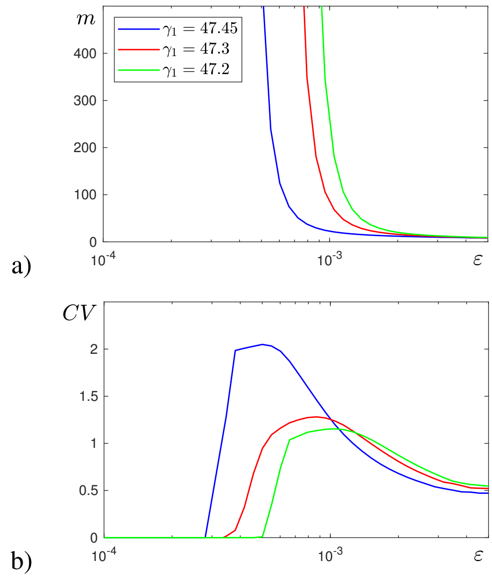

Figure 5. Statistics of interspike intervals in dependence on ε: a) mean values, b) coefficients of variation.

Let us study the probabilistic mechanism of the stochastic generation of large-amplitude oscillations in the model (2). For this purpose, we apply the stochastic sensitivity function technique [Bashkirtseva and Ryashko, 2018; Ryashko, 2018; Alexandrov et al., 2021] which allows us to approximate stationary distribution of random states around attractors.

Suppose that the deterministic system has a stable equilibrium. Then the stochastic sensitivity matrix W of the equilibrium is a unique solution of the matrix equation

$$FW + WF^\top = -S,$$

where F is the Jacobi matrix of the system (1) and S is a matrix which characterizes random disturbances. For the system (2), $S = \mathrm{diag}[0, 0, 1]$.

Eigenvalues and eigenvectors of the matrix W describe a size and direction of dispersion of random states around the deterministic equilibrium. In Fig. 6, eigenvalues of the matrix W for equilibria of the system (1) in dependence on the parameter γ_1 are plotted. One can see

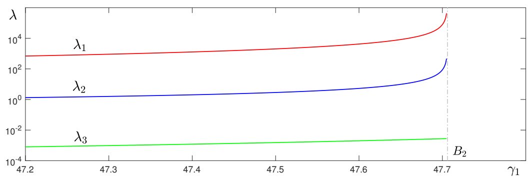

Figure 6. Eigenvalues of the stochastic sensitivity matrix for the equilibria of the system (1).

that the eigenvalue λ_1 is larger than other eigenvalues λ_2 and λ_3 in orders of magnitude. This means that random states are distributed very unevenly around the equilibrium. Thus, one can determine *the principal direction* for deviation of stochastic states. It is the direction of the eigenvector v_1 corresponding to the eigenvalue λ_1.

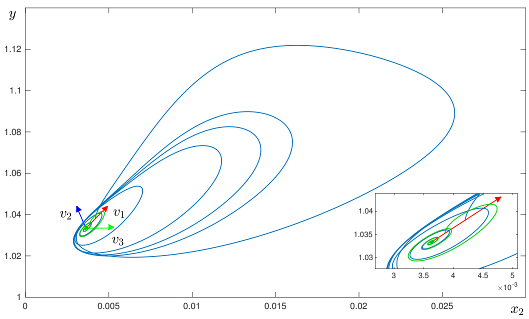

Figure 7. Eigenvectors of stochastic sensitivity matrix and deterministic phase trajectories in projection on the $x_2 - y$-plane for $\gamma_1 = 47.45$.

Fig. 7 shows for $\gamma_1 = 47.45$ the eigenvectors of the stochastic sensitivity matrix for the equilibrium of the system (1) and two deterministic trajectories starting at the points with different deviations from the equilibrium in the principal direction. One of the trajectories goes close to the equilibrium, while another has large-amplitude loops far from it. Thus, one can determine a threshold in the phase space (pseudo-separatrix) which detaches points corresponding to small- and large-amplitude transient processes.

Using the stochastic sensitivity function technique, one can construct the corresponding confidence interval. The ending points of this interval lay on the pseudo-separatrix surface. With these confidence intervals, it is also possible to estimate the critical noise intensity for which large-amplitude oscillations are generated. For $\gamma_1 = 47.45$, we get the value $\varepsilon^* = 0.0005$, and for $\gamma_1 = 47.2$, we get the value $\varepsilon^* = 0.0008$, which agree with the observations obtained with the direct numerical simulations (see Fig. 5).

4 Conclusion

This article is devoted to the problem of revealing the reasons causing complex oscillations in the thermochemical kinetics of combustion processes. In our study, a three-dimensional model describing the combustion process of a mixture of two hydrocarbons was used. It was shown that in the range of parameters, where the original deterministic model has only a stable equilibrium mode, even small random perturbations can generate large-amplitude oscillations. We revealed the probabilistic mechanism of this effect and described the phenomenon of anti-coherence resonance. In analytical study of noise-induced excitement, constructive abilities of the stochastic sensitivity technique and method of principal directions were demonstrated.

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