SIMULATION OF DETONATION INSTABILITIES IN HYDROGEN-AIR MIXTURES

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An important task in assessing the safety of technological processes is to determine the detonation capability of a gas mixture. One of the criteria for the possibility of deflagration transition to the detonation propagation mode is the ratio of the transverse size of detonation cells to the characteristic room size. However, the size of experimental units imposes limitations on the compositions suitable for the study. A numerical study of the characteristics of detonation front instabilities can remove the limitations of the in-situ experiment. Nevertheless, according to [1], the occurrence of instabilities in simulations of detonation propagation does not guarantee correct reproduction of their characteristics obtained in the experiment. As shown in this work, the features of front instabilities depend significantly on the chosen kinetic mechanism. Thus, the development of a numerical model to describe the detonation process in chemically reacting continuous media seems to be relevant.

The system of conservation law equations of the model of a multicomponent single-velocity continuous chemically reacting medium [2], closed by the ideal gas equation of state, is solved during modelling. The reaction rate is determined on the basis of the Arrhenius and acting mass laws [3]. Turbulent quantities are calculated using the Menter SST model [4]. The calculations are performed in the KEDR software package [5] in the finite volume approach with the values placed in the centers of the cells. To increase the approximation order on smooth flow, the flow limiter minmod [6] was used. A modified Kuropatenko method [7] was used on the discontinuous flow. Time integration was carried out by the explicit one-step method of the first order. A stiff-steady solver based on Gear's method [8] was used to solve the stiff system of chemical kinetics equations.

This paper presents intermediate results of the model development, which includes testing various detailed kinetic mechanisms of Ranzi [9], GRI-3.0 [10] and Babushok [11] on experimental data [12, 13, 14] for ignition delay times in the range of temperatures from 850 K to 2200 K and pressures from 1 to 87 atmospheres.

The combustion of a stoichiometric hydrogen-air mixture was modelled using the mechanisms that showed the best agreement with the experimental data. The modelling is performed in a stoichiometric hydrogen-air mixture with direct initiation of detonation. The pressure maxima fields obtained as a result of the simulation are presented in Figure 1.

The results of the analysis of the detonation cell size in the regions highlighted in Figure 1 are presented in Figure 2. For comparison, the size of detonation cells estimated in the experimental work [15, 16] is given.

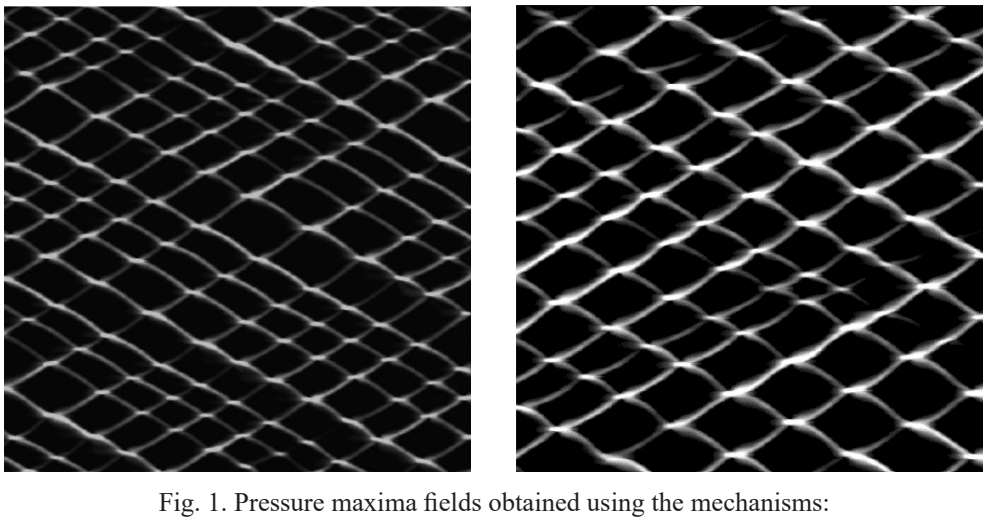
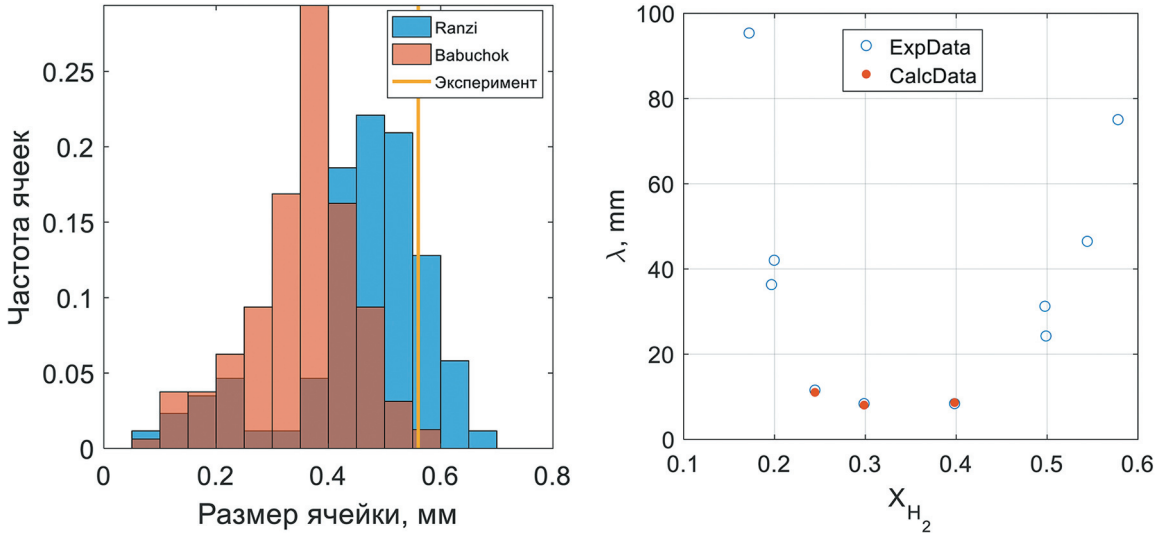


Fig. 1. Pressure maxima fields obtained using the mechanisms:
left – Ranzi [9], right – Babushok [11]



a *b*

Fig. 2. Frequency of occurrence of cells of a certain size (*a*). Experimental data [15].
Size of calculated detonation cells (*b*). Experimental data [16]

In this work, the accuracy of ignition delay modelling using the Ranzi, GRI-3.0, and V. I. Babushok mechanisms has been analysed. It is shown that the Ranzi mechanism provides the closest ignition delays to the experimental data in a wide range of temperatures and pressures. The influence of the detailed kinetic mechanism on the characteristics of detonation front instabilities is demonstrated. The possibility of modelling detonation combustion instabilities using the KEDR software package has been demonstrated.

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