Comparative Analysis of Three Mathematical Models for Hydrogen Ignition

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Introduction

A comparative analysis of three kinetic schemes of hydrogen ignition in oxygen and three gas-dynamic models of the reactive mixture flow behind the initiating shock wave has been performed. An importance of the criterion is shown, which is used to determine the ignition delay time while comparing with experimental data. A numerical analysis of these kinetic schemes has shown that the scheme with 38 reactions of 8 components describes in the best way the experimental data in the temperature range from 900 to 2500 K. It is also shown that at low initial concentrations of hydrogen-oxygen mixture in argon even a simple model, which does not account for the influence of heat release on gas parameters, enables a satisfactory description of the induction period dependencies on temperature. As the initial concentration of reacting components grows, a mathematical model is to be applied, which takes into account the mixture temperature variation.

The problem statement

The problem of physical and mathematical modeling of the behavior of reactive gas mixtures under shockwave loading is important and topical especially in connection with an increased interest in the use of the detonation phenomenon in new engines generations. The use of some sufficiently simple kinetic models of ignition processes and subsequent supersonic combustion of gas mixtures, which nevertheless give credible information about the dynamics of conversions as the reaction develops and adequately describe the process both at the ignition stage and at the combustion stage, appears to be justified. Such integral parameters as the ignition limits and the ignition delay time (the induction period) belong to those basic parameters on the basis of which one can judge about the adequacy of the ignition stage modeling.

The detailed kinetic schemes of [1-3] are used in the present work, and the computed results are compared with experimental data of [4–5] on the ignition delay time dependence on temperature. The computations of hydrogen ignition and combustion behind the shock wave in a mixture $H_2 + O_2 + Ar$ containing from 1 % to 10 % of $H_2 + O_2$ have been carried out at temperatures $800 < T < 2500$ K and pressures $0.3 < p < 5$ atm.

Consider a shock tube filled with a mixture of hydrogen, oxygen, and argon. Let a shock wave (SW) propagate in the mixture. Under certain conditions for the SW Mach number the mixture parameters may exceed the critical values, and the ignition occurs.

The mixture dynamics is governed in the one-dimensional formulation by the non-equilibrium gas dynamics equations augmented by the gas mixture equation of state and the kinetic equations of chemical conversions. This makes it possible to compute the pattern of the shock wave propagation in the duct upon formulation of the corresponding initial- and boundary-value problem with regard for possible chemical conversions. The given model will be termed the nonstationary model.

If the process of the mixture ignition in the shock tube is assumed steady, and a passage is made to a self-similar variable related to the SW front coordinate $\zeta = x - Dt$, where D is the

SW velocity, then the problem of the progressive ignition wave reduces to the solution of an ordinary differential equation for velocity:

$$\frac{du}{d\zeta} = \frac{\dfrac{R}{c_v M_{\text{см}}} \sum\limits_{\alpha=1}^{\mu} \dfrac{d\xi_\alpha}{dt} \left(c_{v_\alpha} T + h_{0_\alpha} - c_{p_\alpha} T_{00} \right) - RT \sum\limits_{\alpha=1}^{\mu} \dfrac{1}{M_a} \dfrac{d\xi_\alpha}{dt}}{u^2 - c_f{}^2},$$

here $M_{\text{см}}$ and c_f are the molecular weight and the frozen sound velocity in mixture, R is the universal gas constant. The values of the remaining gas-dynamic parameters in the chemical relaxation zone are found from the laws of conservation of mass, momentum, and energy. Completing this equation by the chemical kinetics equations we obtain a system of ordinary differential equations for which a Cauchy problem is posed with the initial conditions for mass concentrations $\xi_\alpha \big|_{\varsigma=0} = \xi_{\alpha 0}$, and the initial condition for velocity $u\big|_{\varsigma=0} = u_f$, where u_f is the velocity behind the front of the frozen SW. This model will be termed the stationary model.

In the case when an inert gas occupies the most part of the mixture (up to 90%), then the temperature variation due to heat release and, consequently, the variation of other gas dynamic parameters may be neglected, and the computation can be carried out in the isothermal approximation. This model will be termed the isothermal model.

The detailed kinetic mechanisms [1-3] have been used to describe the chemical conversions, which involve 60, 42, and 38 direct and inverse reactions, respectively, of 8 chemical components: H_2, O_2, H_2O, OH, H, O, HO_2, and H_2O_2. The constants of the rates of direct and inverse reactions are presented in [1-3].

Results and discussion

An important issue is here the choice of a criterion for the determination of the ignition moment of time. Figure 1 shows the dependencies of the ignition time delay (t_{ign}) computed by three most frequently used criteria versus the temperature behind the shock wave. The maximum of the OH radical, the maximum of the growth of the OH radical, and the maximum of temperature growth were used as the criteria. The computations have been performed by using the stationary model and the kinetic mechanism [1]. The computed results are compared with the experiment of [5]. The results of determining $t_{ign}(T)$ by different techniques can be seen from the figure to differ considerably (by 2 – 3 times) from one another.

The data computed by three kinetic schemes and the experimental data of [4, 5] on the dependence of the ignition delay time (t_{ign}) ($W^0_{O_2}$ is the initial molar volume concentration of O_2) versus the temperature behind the SW is presented in Fig. 2. All the kinetic schemes are seen to predict correctly the value of t_{ign} in the temperature range $1000 < T < 2500$K and underesitimate t_{ign} at $T < 1000$ K. The kinetic schemes of [1, 2] yield practically the same results, and t_{ign} obtained by using the mechanism of [3] differs not very significantly from them for $T > 2000$ K. It is obvious that a change of the reaction mechanism occurs in the temperature range $T < 1000$ K, and a correction of the rates constants is necessary to ensure a better agreement with experiment of [4].

We now proceed to a comparison of different gas dynamic models of the mixture ignition with one another. The values of t_{ign} are presented in Fig. 3 versus the temperature behind the SW, which were obtained by using three different gas dynamic mathematical models of the process. The kinetic scheme of [3] was used as in the foregoing case. The computed results are presented for the initial concentration of 2.5% of $2H_2+O_2$. Solid lines show the predictions of the isothermal and stationary models, and the dots refer to the computed data obtained on the basis of the nonstationary model of the process. The proximity of the results computed by all three models is seen from Fig. 3. This also enables us to assert that the ignition of the reacting mixture of hydrogen and oxygen with a large admixture of an inert gas at a shockwave interaction can be described with the aid of the isothermal mathema-tical model if the concentration of reagents does not exceed certain limiting value $\xi^{*}_{H_2+O_2 0}$.

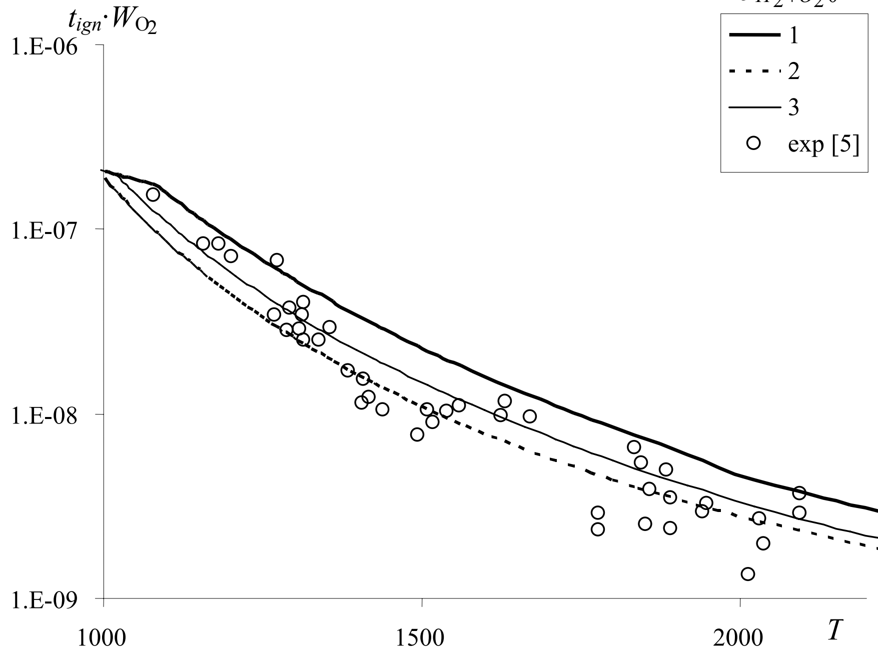

Fig. 1 Comparison of the ignition criteria (1 — the maximum of the OH concentration, 2 — the maximum of the OH concentration growth, 3 — the maximum of the temperature growth).

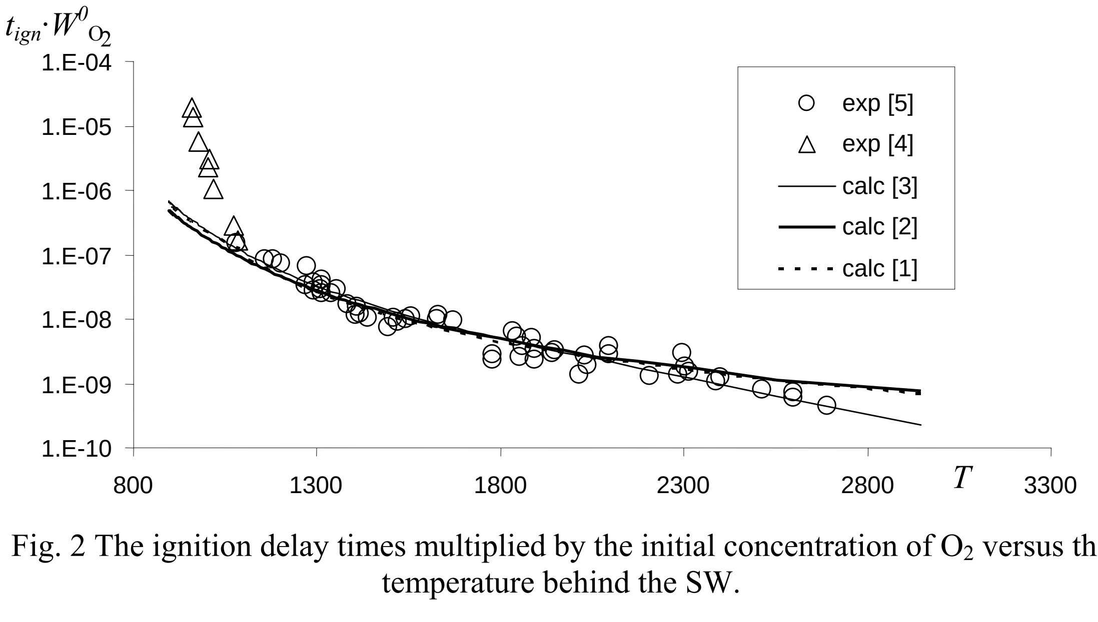

Fig. 2 The ignition delay times multiplied by the initial concentration of O_2 versus the temperature behind the SW.

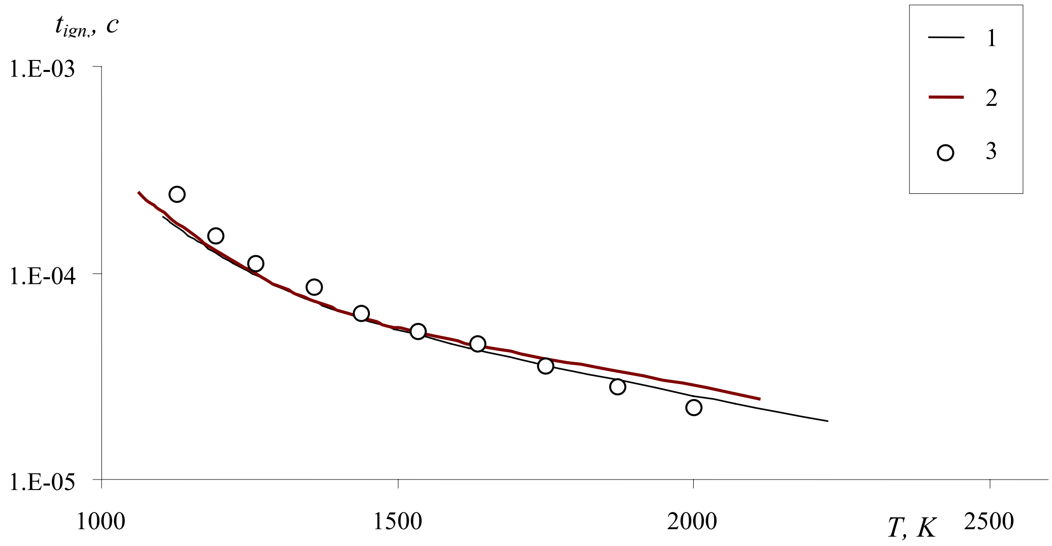

Fig. 3. Comparison of the ignition delay times obtained by three different models of the process gas dynamics (1 the isothermal model, 2 the stationary model, 3 the nonstationary model)

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