Intensification of shock-induced combustion by electrical-discharge-excited oxygen molecules

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1 Introduction

The arranging of the effective fuel burning in the high velocity flow is one of the most complex problems in the prospective propulsion systems. One of the promising concepts extensively investigated during last years is based on the use of shock wave to induce the stable combustion or to arrange an oblique detonation wave (ODW) [1, 2]. Stabilization of an ODW in the supersonic flow may be attained by the usage of a sharp wedge body. Despite the fact that shock wave facilitates the ignition in supersonic flow and makes it possible to provide the stable combustion, the distance at which the ignition occurs in practically interested cases is too large and cannot be suitable for modern or prospective propulsion systems.

Therefore, it is very useful to consider different approaches to enhance the shock-induced combustion or detonation wave formation in a supersonic flow. This paper deals with the analysis of the kinetic mechanism of the enhancement of shock induced combustion and initiation of the detonation wave over the wedge due to activation of oxygen molecules in electrical discharge.

2 Intensification of ignition and combustion behind an oblique shock wave

Consider shock-initiated combustion in a supersonic flow. The flow scheme is presented in Fig. 1. Molecular oxygen and hydrogen flow in inner and outer coaxial channels, respectively, and the oxygen molecules are excited by electrical discharge. The parameters of undisturbed flow vary over the following limits: temperature \( T_0 = 300 \) K, pressure \( P_0 = 10^3–10^5 \) Pa, and Mach number \( M_0 = 4–6 \). For such parameters, the characteristic time of mixing of the hydrogen and oxygen plasma is no greater than \( 10^{-4} \) s. After mixing, the homogeneous flow consisting of molecular hydrogen and components produced in the discharge zone interacts with a stationary shock wave the front of which makes angle \( \beta \) with the velocity vector of the incoming flow. The gas velocity behind the shock remains supersonic.

Recent theoretical and experimental researches of processes taking place in an oxygen plasma produced by a semi-self-maintained discharge have shown that, with the above parameters of the flow, the concentration of electronically excited molecules \( O_2(a^1\Delta_g) \) may be sufficiently high (up to 5% even at atmospheric pressure). The parameters and composition of the discharge plasma depend on the initial temperature and pressure in the medium, reduced electric field \( E/N \) (\( E \) is the electric field strength, \( N \) is the number density of molecules), and specific energy \( E_s \) put into the gas.

To describe the ignition/combustion in \( \text{H}_2-\text{O}_2 \) mixture behind the shock wave a thermally non-equilibrium kinetic model was developed. This
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model is based on our previous works [3, 4] and assumes that rotational and translational degrees of freedom of molecules are in a thermodynamic equilibrium and in the each vibrational mode the Boltzmann distribution is appeared. The reaction mechanism includes reversible chemical reactions with participation of H, O, OH, H₂O, H₂, HO₂, H₂O₂, O₃, and O₂(\(^{X_{3}}\Sigma^+_g\)), O₂(\(^{a^1}\Delta_g\)), O₂(\(^{b^1}\Sigma^+_g\)) species, the processes of V–V' exchange between the modes of H₂O, H₂, O₂(\(^{X_{3}}\Sigma^+_g\)), O₂(\(^{a^1}\Delta_g\)), O₂(\(^{b^1}\Sigma^+_g\)), OH, HO₂, H₂O₂, and O₃ molecules, and the processes of V–T relaxation of the energy of these molecules. Note that applied kinetic model allows to predict properly the measurements of the induction zone length behind the front of shock wave at temperatures just alter the front \(T \geq 800\) K and to describe the experimental data on the enhancement of combustion of H₂–O₂ mixture due to excitation of oxygen molecules to the singlet electronic state \(^{a^1}\Delta_g\) in electrical discharge obtained recently in [5].

The set of equations describing the flow of a vibrationally nonequilibrium reacting gas behind the shock front in the \(x\) direction includes the continuity equation, momentum and energy equations, equations for component concentrations, and equations for the mean number of vibrational quanta stored in each mode of molecular components in a reacting medium.

Consider the kinetics in a stoichiometric H₂–O₂ mixture downstream the shock front when molecular oxygen is activated by an electrical discharge with \(E/N=1.1 \times 10^{-16}\) V cm\(^{-2}\) versus the usual case, where the mixture is heated by the discharge energy. Figure 2 plots the molar fractions of the mixture components against distance \(x\) from the shock front for the cases under study at the same specific energy put into the gas, \(E_s=3 \times 10^{-2}\) J/cm\(^3\) and \(P_0=10^4\) Pa. At such discharge parameters the predicted composition of oxygen discharge plasma is following: 0.958 O₂(\(^{X_{3}}\Sigma^+_g\)), 0.0322 O₂(\(^{a^1}\Delta_g\)), 7.66 \times 10^{-3} O₂(\(^{b^1}\Sigma^+_g\)), 1.2 \times 10^{-3} O(\(^3\)P), and 3.52 \times 10^{-5} O₃; the vibrational temperature of O₂(\(^{X_{3}}\Sigma^+_g\)) is 984 K.

In the first case, the gas temperature behind the mixing zone is 354 K, in the second case 429 K. In going through the shock front, the temperature of the mixture rises, respectively, to 613 and 742 K. However, although the temperature of the mixture behind the front is much smaller in the case of oxygen activation in the discharge, it inflames much faster than in the case of mere heating. In the first case, the length of the induction zone is \(L_{in}=15\) cm; in the latter \(L_{in}=107\) m. Note, in the ordinary H₂–O₂ mixture with \(T_0=354\) K (the temperature of the discharge plasma at \(E_s=3 \times 10^{-2}\) J/cm\(^3\)) and the same \(P_0\) and \(M_0\), the induction zone is as long as 600 m; that is, excitation of oxygen molecules by an electrical discharge makes it possible to shorten the induction zone length by 4000 times at moderate temperatures behind the shock front (\(T_1 \approx 600\) K).

Acceleration of inflammation by exposing the O₂ flow to a tailored electrical discharge is explained by enhancement of chain reactions owing to presence of vibrationally excited and electronically excited O₂ molecules and a small amount of O atoms and O₃ molecules in the...
oxygen plasma. The curves in Fig. 2 indicate that, in the case of discharge activated O₂ molecules, OH radicals and H atoms rapidly arise behind the shock front and the concentrations of O₃ and O₂(\textit{b}₁\textit{Σ}⁺\textit{g}) start decreasing almost right off. When the mixture is heated by the electrical discharge with \(E_s=3\times10^{-2}\ J/cm^3\) \((T_0=429\ K)\), the highest concentrations at the initial stage of oxidation are observed for HO₂, H₂O, and H. This means that the pathways of chain mechanism differ in these two cases.

Computations showed that low-temperature inflammation of the mixture with electronically and vibrationally excited O₂ molecules makes it possible to raise the efficiency of conversion of the reactant chemical energy to heat compared with the conventional way of combustion initiation by heating. The energy gain in terms of energy converted to heat during combustion may mount to 30%. In the case of low-temperature combustion initiation, higher values of the temperature and pressure of combustion products are also achieved.

3 Initiation of detonation shock wave by electrical-discharge-excited oxygen molecules

The schematic of the flow configuration is given in Fig. 3. A gaseous fuel (H₂) is mixed in a narrow near-axis region with the flow of molecular oxygen activated by the electrical discharge. The radial dimension of this region is limited and its radial boundary is denoted as \(y_e\). At \(y>y_e\), the oxygen flow is not activated and the H₂-O₂ mixture contains only O₂ molecules in the ground electronic state \(X^3\Sigma^−\).

Flow parameters prior to mixing are: temperature \(T_0=400-600\ K\), pressure \(P_0=10^3-10^4\ Pa\), and Mach number \(M_0=4-6\). The reactive flow with mixing layer is treated within the parabolized Navier-Stokes equations.

Figure 4 shows the predicted pressure field in the flow at \(M_0=6\), \(T_0=600\ K\), and \(P_0=5\times10^3\ Pa\) for the stoichiometric H₂-O₂ mixture and \(E_s=0\) \((y_e=0)\) for two cases: (a) the model takes into account the delayed excitation of molecular vibrations of reactants behind the shock front (thermally nonequilibrium model); (b) the model does not take into account these phenomena (conventional thermally equilibrium model).

Under the flowing of a wedge by supersonic flow the primary oblique shock wave (OSW) centered on the obstacle leading edge forms. The ignition of the mixture occurs behind the shock front near the wedge surface. Depending on longitudinal coordinate, three characteristic regions in the flow can be identified (see Figure 4). Region 1 is the induction region, where the flow parameters behind primary OSW front are unchanged. The length of this region is denoted as \(L_{ign}\). Region 2 is the transition zone, where the ignition of the mixture occurs. Heat-release during combustion process in this zone results in a generation of compression waves, which produce the primary detonation wave. The length of this region is denoted as \(L_t\). The interaction of this detonation wave with the OSW is followed by the main ODW formation in Region 3. The distance from the wedge apex to the beginning of this zone is denoted as \(L_d\) \((L_d=L_{ign}+L_t)\).

It is worth to note that even thermally equilibrium model predicts for the homogeneous flow of a stoichiometric H₂-O₂ mixture with \(M_0=6\), \(P_0=5\times10^3\ Pa\), \(T_0=600\ K\) very large values of the ignition and detonation zone lengths, \(L_{ign}=5.7\ m\) and \(L_d=7.7\ m\). Therefore it is very important to reduce significantly both \(L_{ign}\) and \(L_d\) values. As was demonstrated above the acceleration of chemical reactions in the induction region may be occurred by excitation of oxygen molecules to the singlet electronic states \(a^1\Delta_g\) and \(b^1\Sigma^+\) in electrical discharge even if the input energy is low \((E_s\sim3\times10^{-2}\ J/cm^3)\).

Consider now a case where the mixing of oxygen activated in the electrical discharge and the outer H₂-O₂ flow occurs in the region over the wedge surface and the temperatures of the inner oxygen plasma flow and the outer H₂-O₂.
flow are different. In this case, the mixing layer beginning at the wedge apex \((x=0)\) spreads along the stream with the axial coordinate \(y=y_e\) and interacts with the OSW front at a certain distance from the wedge apex. The latter depends on \(y_e\) and \(\beta\).

At low temperature of the outer \(H_2-O_2\) flow \(T_{out}=400\) K and \(E_s=0\) there is no ignition in the flow behind the OSW and therefore, no detonation. Excitation of oxygen molecules by the electrical discharge makes it possible to obtain ignition and detonation in the flow over the wedge. The increase in the discharge energy leads to the decrease in the distance of detonation formation. The interesting trend is found for this case: decreasing the discharge zone height, \(y_e\), leads to decreasing \(L_d\). In this case, ignition starts in the region where the mixing layer interacts with the OSW. This is seen from the pressure fields displayed in Fig. 5 when the temperature in the inner oxygen plasma flow is 354 K and the temperature in the outer \(H_2-O_2\) flow is only 400 K.

One can conclude that for detonation initiation, it is sufficient to activate oxygen molecules in a narrow near-axis layer adjacent to the wedge apex. Thus, there is a possibility to obtain the stabilized detonation in a supersonic flow at the distance \(~1\) m from the wedge apex by depositing relatively low discharge energy to the gas.

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