Oxyhydrogen Ignition and Flame Propagation Under Cryogenic Temperatures

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Summary: One-dimensional numerical calculations were performed for ignition and flame propagation of oxyhydrogen mixtures under cryogenic conditions. Three aspects on ignition problems were studied; 1) an effect of ambient temperature on the minimum ignition energy, 2) an effect of initial pressure on the minimum ignition energy per mass, and 3) an effect of energy deposit rate on the minimum ignition energy.

Introduction

Ignition and flame propagation of oxyhydrogen mixtures under cryogenic conditions have been an important subject for rocket combustion, combustion of hydrogen as clean fuel and their safety problems for a long time. However, even the ignition problem has not been studied enough, due to the coupling structure among transport processes, chemical reaction and fluid dynamics. The present study deals only with the fundamental aspects of oxyhydrogen ignition and flame propagation in cryogenic environments.

Recent liquid oxyhydrogen ignition tests [1] revealed that there existed ignition failures under certain cryogenic conditions. Several factors can be considered to explain these failures; 1) a relation between the rate of energy deposit and the minimum ignition energy is affected, 2) a relation between the heat release by combustion and the minimum ignition energy, 3) an effect of shock or detonation waves on the ignition and flame propagation, 4) icing of reaction products on the spark electrode or in gas phase, etc. The first problem has been discussed by Bach et al. [2] and Lee, et al [3] regarding a detonability limit; the rate of energy deposit $\dot{E}_s$ increases with decreasing pressure or increasing induction delay (ignition time). Evidently, this implies that the rate of energy deposit increases when the minimum ignition energy increases. The second problem emerges after an ignition occurs, but is related with the first problem. Since an ambient condition is cryogenic, the heat release by chemical reaction has to compete with the heat conduction in the ignition as well as in the flame propagation problems.

The third problem explains the energy deposition coupled with the fluid mechanics, as discussed by Bach et al. [4]. The decoupling of shock and reaction zone occurs in a subcritical energy regime, whereas the initially overdriven spherical detonation decays asymptotically to the C-J state in a supercritical energy regime, and in a

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critical energy regime the decoupling first occurs, followed by the re-establishment of a highly asymmetrical multihead detonation. The fourth problem is a technical but serious one. The icing phenomena produce occasional ignition failures using the same spark plug, for example. In view of the available experiments, it is known that the minimum ignition energy is strongly dependent not only on the properties of a gas mixture, but also on the characteristic features of igniters [3].

Numerical Analysis

Numerical calculations were carried out for the problem 1) discussed in the previous section, using the HCT program [5]. This program implicitly solves one-dimensional nonsteady differential equations for the conservation of mass, momentum, energy and chemical species taking account of a full chemical mechanism (Table I).

Table I   Hydrogen-oxygen reaction mechanism. Reaction rates in cm³-mole-sec-kcal units, $k = AT^n \exp(-E_a/RT)$

Reaction		Forward rate			Reverse rate		
		$\log A$	n	E_a	$\log A$	n	E_a
1.	$H + O_2 \longrightarrow O + OH$	14.27	0	16.79	13.17	0	0.68
2.	$H_2 + O \longrightarrow H + OH$	10.26	1	8.90	9.92	1	6.95
3.	$H_2O + O \longrightarrow OH + OH$	13.53	0	18.35	12.50	0	1.10
4.	$H_2O + H \longrightarrow H_2 + OH$	13.98	0	20.30	13.34	0	5.15
5.	$H_2O_2 + OH \longrightarrow H_2O + HO_2$	13.00	0	1.80	13.45	0	32.79
6.	$H_2O + M \longrightarrow H + OH + M$	16.34	0	105.00	23.15	−2	0.00
7.	$H + O_2 + M \longrightarrow HO_2 + M$	15.22	0	−1.00	15.36	0	45.90
8.	$HO_2 + O \longrightarrow OH + O_2$	13.70	0	1.00	13.81	0	56.61
9.	$HO_2 + H \longrightarrow OH + OH$	14.40	0	1.90	13.08	0	40.10
10.	$HO_2 + H \longrightarrow H_2 + O_2$	13.40	0	0.70	13.74	0	57.80
11.	$HO_2 + OH \longrightarrow H_2O + O_2$	13.70	0	1.00	14.80	0	73.86
12.	$H_2O_2 + O_2 \longrightarrow HO_2 + HO_2$	13.60	0	42.64	13.00	0	1.00
13.	$H_2O_2 + M \longrightarrow OH + OH + M$	17.08	0	45.50	14.96	0	−5.07
14.	$H_2O_2 + H \longrightarrow HO_2 + H_2$	12.23	0	3.75	11.86	0	18.70
15.	$O + H + M \longrightarrow OH + M$	16.00	0	0.00	19.90	−1	103.72
16.	$O_2 + M \longrightarrow O + O + M$	15.71	0	115.00	15.67	−0.28	0.00
17.	$H_2 + M \longrightarrow H + H + M$	14.34	0	96.00	15.48	0	0.00
18.	$O_2 + H_2 \longrightarrow OH + OH$	14.90	0	44.70	13.44	0	26.86
19.	$O + OH + M \longrightarrow HO_2 + M$	17.00	0	0.00	21.92	−1	65.85

Oxyhydrogen Ignition

The chemical kinetic mechanism of oxyhydrogen ignition is considered to consist of 8 species and 19 elementary reactions illustrated in Table I. The present problem is described in the following: An equi-molar oxyhydrogen mixture is ignited at the left end wall of a cylinder, the cross sectional area of which is 1 cm² while its length 10 cm, resulting in the total volume $v = 10$ cm³. The initial conditions are $P_0 = 260$ Torr and $T_0 = 100$ K, yielding the total mass of the contained

gas $M_t = 7.08 \times 10^{-3}$ grams and the mass density $\rho_0 = 7.08 \times 10^{-4}$ g/cm^3. By assuming the adiabatic walls on both ends of the cylinder, the loss of applied energy is prevented. Ignition energy is supplied in the form of a volumetric heat source, localized within $V_0 = 0.04$ cm $\times 1$ cm^2 adjacent to the left wall boundary. Currently, the strength of the volumetric heat source is chosen as $\dot{E}_v = 7.327$ J/mm^3/sec $=$ const. The amount of energy addition is controlled by the duration τ_{ig} of the volumetric heat source application before ignition starts. As shown in Fig. 1, τ_{ig} is determined from the evolution of the H_2O mole fraction within V_0; the intersection of the maximum slope with the time axis is chosen as $\tau_{ig} = 1.064 \times 10^{-4}$ sec. Thus, the specific energy deposit $E_{total} \equiv \dot{E}_v \times \tau_{ig} = 0.78$ mJ/mm^3. The rate of energy deposit $\dot{E}_s \equiv \dot{E}_v \times 0.04$ cm $= 7.327 \times 10^3$ J/cm^3/sec $\times 0.04$ cm $= 293$ J/cm^2/sec.

A moving grid is used to integrate physical values accurately, especially, in the flame zone. Three aspects are investigated in this report; (1) a relation between minimum ignition energy and initial temperature, (2) a relation between minimum ignition energy per mass and initial pressure, and (3) a ralation between minimum ignition energy and rate of energy deposit. From the numerical analysis, the one-demensional minimum ignition energy is defined by the ignition time τ_{ig} multiplied by the rate of energy deposit $\dot{E}_s$.

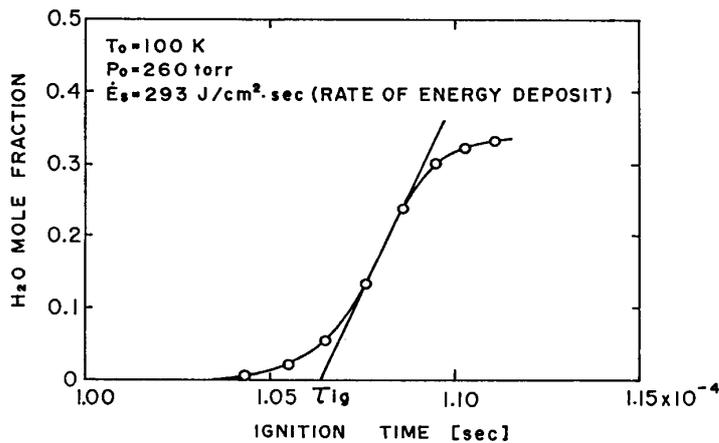

Fig. 1. Determination of ignition time

(1) The Effect of Ambient Temperature

Meanwhile, our experimental result [6] showed a strong dependecy of minimum
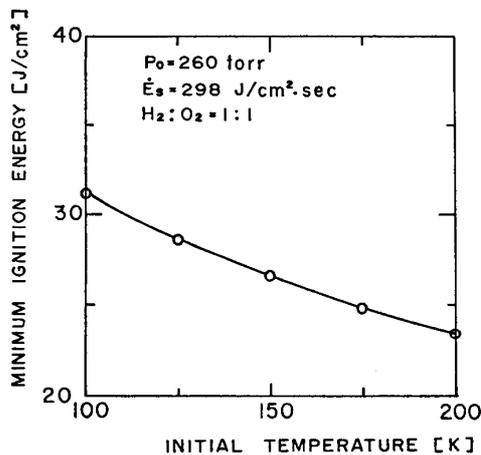

Fig. 2. The effect of ambient temperature

ignition energy on temperatures under cryogenic conditions. In other words, a higher minimum ignition energy was apparently required to ignite the mixture at a lower cryogenic temperature in the experiment. However, the computational result in Fig. 2 showed that the slope of the dependency of minimum ignition energy on temperature is less steep. This is because in the present calculation only the physico-chemical properties of gas is influenced by the cryogenic condition of ambient atmosphere. The effects of phase change, e.g., icing may be necessary to properly interpret the experimental results in an actual applicational situation, i.e., liquid propellant rocket ignition.

(2) The Effect of Initial Pressure

As illustrated in Fig. 3, the calculated minimum ignition energy per unit mass increases, when the initial pressure is decreased, until it apparently approaches infinity at a critical limiting initial pressure between 20 and 30 Torr. Instead of the minimum ignition energy, the energy per unit mass is utilized to avoid the effect of density change caused by the change of initial pressure. The existence of infinity implies that below the critical limiting pressure transport phenomena dominate chain branching reactions due to the longer mean free path and stop building up an exothermic center. The tendency of minimum ignition energy increase at lower initial pressures is also observed by Bach et al. [2] in the direct initiation of diverging detonations, although unlike the present oxyhydrogen ignition phenomenon the detonation initiation is more related with sufficiently strong shock wave formation.
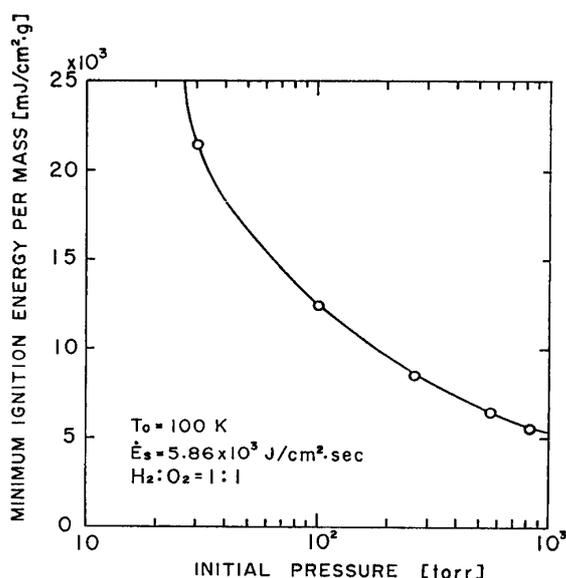

Fig. 3. The effect of initial pressure

(3) The Effect of Energy Deposit Rate

In the present calculation, the rate of energy deposit $\dot{E}_s$ was changed while retaining the amount of ignition energy $E_s \equiv \dot{E}_s \times \tau_{ig}$. It was found out, as shown in Fig. 4, that the minimum ignition energy decreases with decreasing rate of energy deposit. Specifically, there exists a limiting minimum ignition energy, E_s
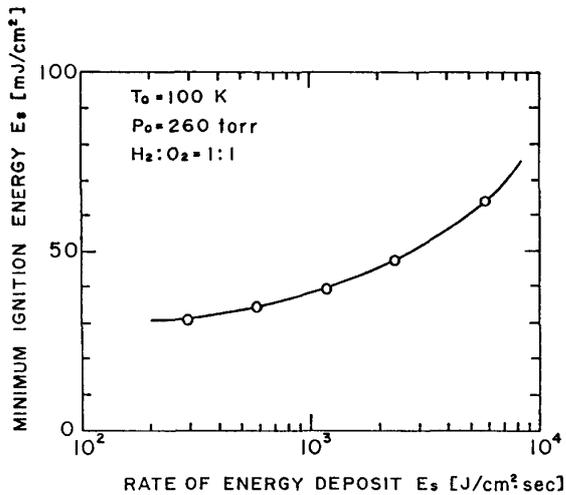
Fig. 4.   The effect of energy deposit rate

$=30 \, \text{mJ/cm}^2$, when $\dot{E}_s$ is reduced down to $10^2 \, \text{J/cm}^2 \cdot \text{sec}$. This limiting value can indeed be considered as the minimum ignition energy to ignite a given gas mixture. According to the above results, it should be noted in the experimental study of minimum ignition energy that the rate of energy deposit $\dot{E}_s$ has to be adjusted properly in order to find out the minimum value for the ignition of a given mixture.

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