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Shock tube study on ignition delay of hydrogen and evaluation of various kinetic models

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ABSTRACT

H_2/O_2 chemistries are of great crucial for all hydrocarbon and syngas oxidations. Recent study showed that presence of residual H-atom in shock tubes may heavily influences experimental determination of ignition delay times in H_2/O_2 mixtures. Although numerous studies of hydrogen ignition delay times were reported, none of them discussed the residual H-atom in their studies which may impact the accuracy of their measurements. In this study, a systematic measurement related to the ignition delay times were conducted for H_2/O_2 mixtures diluted with argon over the temperatures from 850 K to 1500 K, the pressures from 1.2 to 16.0 atm, and the equivalence ratios of 0.5, 1.0 and 2.0. Special attentions were paid to eliminate the influence of residual H-atom on ignition delay time and the calculation showed that the residual H-atom in current shock tube shows no obvious effect on ignition delay time, which guarantees the present data more convincing. The measurements showed that the hydrogen mixtures have different global activation energies under different pressures. Thus, correlations were derived under different pressures based on all experimental data, which fit fairly well with the experimental data. A couple of detailed kinetic models from literature were validated against the present experimental results. The result shows that the mechanism of Kéromnès-2013 yields the best agreement with data from shock tube experiments at various pressures up to 16 atm, while Davis-2005, GRI 3.0, SanDiego-2011 and Li-2004 mechanisms present significant poor predictions at higher pressures. This investigation is contrary to the previous studies. Reaction pathway and sensitivity analysis indicated that reaction R10: $H + O_2$ (+M) <=> HO_2 (+M) is of significant important pressure-dependent reaction in controlling of hydrogen oxidation. It is inferred that significant differences of their rate constants among various mechanisms induce the difference of performance on hydrogen ignition predictions.

Introduction

Studies on clean-alternative fuels have been motivated by environmental and energy supply issues. Among various alternative fuels, hydrogen is regarded as a promising alternative fuel in transportation, heating, and power plants in the future due to some favorable combustion characteristics [1,2]. The main property of hydrogen relevant to its engine compatibility is its high flame speed, resulting in broad burn

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Table 1 – Composition of the test mixtures.

Mixture	ϕ	% H_2	% O_2	% Ar
2	0.5	3.472	3.472	93.056
5	1	5.917	2.959	91.124
8	2	9.132	2.283	88.584

limit and can increasing the fraction of exhaust gas recirculation. In addition, hydrogen is the most abundant element in the universe without any carbon, leading to essentially no carbon related pollution. Moreover, H_2/O_2 chemistries play of important part in every hydrocarbon and oxygenate oxidation mechanism because it contains many important elementary reactions involving H, O, OH, HO_2, H_2O, and H_2O_2 that play significant roles in all stages of hydrocarbon oxidation [3]. Therefore, an accurate and reliable kinetic mechanism for hydrogen that can represent its combustion characteristics over a wide range of conditions is historically pursued.

Numerous hydrogen oxidation mechanisms have been reported in the past decades [4–15], which were motivated by the substantial progress achieved in accurate measurement of the elementary reaction rates and thermodynamic properties. The kinetic mechanisms of Ó Conaire et al. [5] and Li et al. [6] were refined by incorporating the best up-to-date available kinetic and thermos data into the mechanism of Mueller et al. [4]. Davis et al. [7] proposed a detailed H_2/CO mechanism based on H_2/CO sub-mechanism of the GRI-Mech version 3.0 [16] by considering the recent revisions in the rate coefficient of H + O_2 (+M)<=> HO_2 (+M), its third-body efficiencies, and the enthalpy of formation of the OH radical. Zsély et al. [8] refined the H_2/CO sub-mechanism of the Leeds methane oxidation [17] mechanism by incorporating the latest rate constant evaluations [18]. Special attention has been focused in this work [8] to the uncertainties of the calculation caused by the uncertainties in the rate constants. A detailed H_2/CO mechanism with rate parameters for elementary steps in the

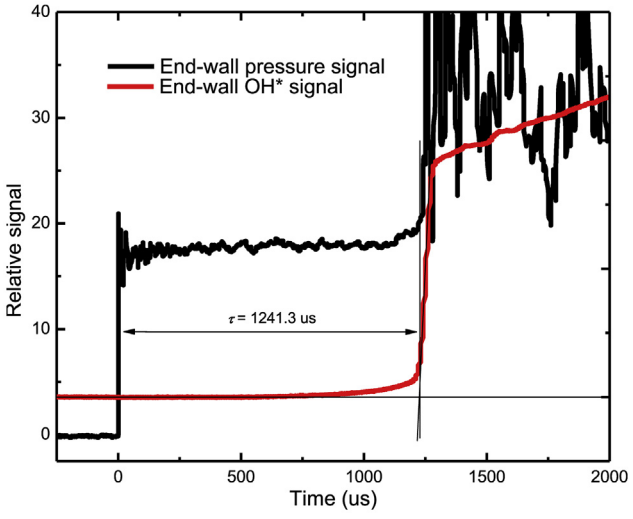

Fig. 1 – Typical end-wall pressure and OH* chemiluminescence measurements the corresponding ignition delay time for a stoichiometric $H_2/O_2/Ar$ mixture at 16.63 atm and 1082.4 K.

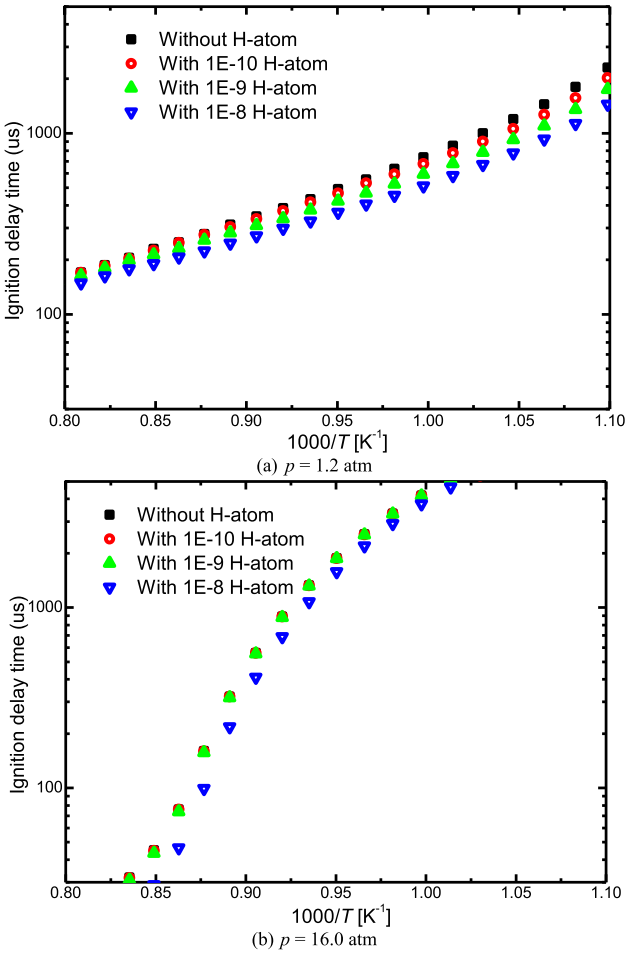

Fig. 2 – The effect of residual H-atom on simulations at $p = 1.2$ and 16.0 atm for the stoichiometric $H_2/O_2/Ar$ mixture using the mechanism of Kéromnès et al. [14].

mechanism for hydrogen and to deletion of a hydrogen initiation step and addition of an initiation step for carbon monoxide was proposed by Saxena et al. [9]. Konnov et al. [11]

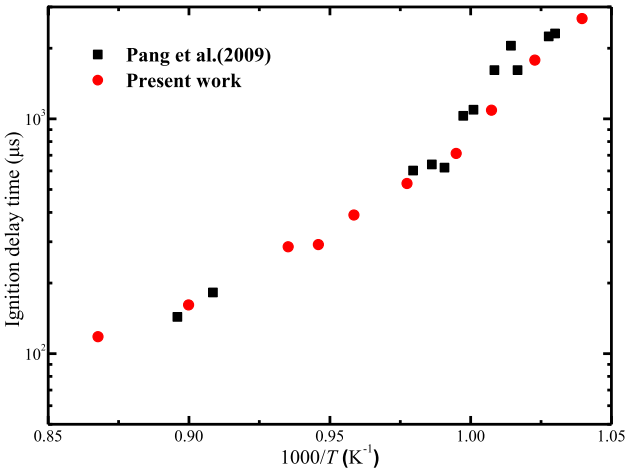

Fig. 3 – Comparison between present measured data and the measured data from reference for 4%H_2/2%O_2/94%Ar at $p = 3.5$ atm and $\phi = 1.0$.