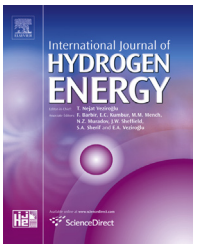
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2016) 1–16

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he



Construction of one-step H_2/O_2 reaction mechanism for predicting ignition and its application in simulation of supersonic combustion

Bing Wang [a], *Wei Wei* [a], *Suna Ma* [a], *Gao Wei* [b,c,*]

[a] *School of Aerospace Engineering, Tsinghua University, Beijing 100084, China*
[b] *School of Chemical Machinery and Safety Engineering, Dalian University of Technology, Dalian, Liaoning 116024, China*
[c] *Institute of Fluid Science, Tohoku University, Sendai, Miyagi 980-8577, Japan*

ARTICLE INFO

Article history:
Received 11 August 2015
Received in revised form
4 September 2016
Accepted 5 September 2016
Available online xxx

Keywords:
One-step mechanism
Ignition delay time
Hydrogen combustion
Supersonic mixing layer
CFD

ABSTRACT

This study developed a method to establish a one-step global reaction mechanism for predicting the ignition delay time. The activation energy database applied in 850–1800K temperature, 0.1–100 atm pressure and a wider excess air coefficient within the range of flammable limit was constructed and the one-step reaction mechanism was then obtained for a specified chemical reaction state through a look-up or Lagrange interpolation technology. The present one-step global mechanism is able to predict the accurate ignition delay time compared with the detailed mechanism, and is superior to the other available reduced mechanisms. Coupled to a high-order in-house Computational Fluid Dynamics (CFD) code, the current reaction mechanism is successfully applied to numerical simulations of supersonic chemically reacting mixing layers under different flow conditions. The numerical predictions of supersonic combustion process, ignition position as well as averaged flow fields, using the present mechanism are comparable to the results using the detailed mechanism. Therefore, this simplified reaction mechanism is suitable for fast simulation-based designs in industrial.

Introduction

The accurate prediction of the ignition delay time is always an important issue involved in the combustion system, which has attracted the attention from academic and industry scientists [1]. In the possible fuels of aerospace engines, hydrogen is a good choice because of its clean-burning (the combustion product is water), good cooling performance (its specific heat is an order of magnitude larger than typical hydrocarbon fuels), wide flammable limit (the explosive limit is changed from 4 to 75% in air), low ignition energy (0.017 mJ) and so on, even if it has the disadvantages of low density specific impulse and special handling of storage materials. Therefore, the accurate prediction of hydrogen/air combustion process is the key to the design of combustion chambers of engines fueled by hydrogen.

* *Corresponding author*. School of Chemical Machinery and Safety Engineering, Dalian University of Technology, Dalian, Liaoning 116024, China.
Fax: +86 411 84986501.
E-mail address: gaoweidlut@dlut.edu.cn (G. Wei).

http://dx.doi.org/10.1016/j.ijhydene.2016.09.010
0360-3199/

The combustion process of hydrogen and air can be well calculated using the detailed reaction mechanism in perfectly stirred reactor or simple flow models. The predictions can present the ignition delay time, the flame propagation speed and some other important parameters. However, these combustion parameters require a large correction for further practical applications due to the over-simplification of flow process. The practical correction is usually empirical. Certainly, the combustion characteristics can be obtained using detailed mechanisms in the actual reacting flow by means of Computational Fluid Dynamics (CFD) technology [2]. This approach costs amount of computing resources, and has extremely high requirements in the robustness and efficiency of numerical algorithms. Thus, the CFD coupled with detailed chemistry is quite limited currently in engineering practice. Coupling a reduced one-step global chemical reaction to a CFD solver of complex flow is very desirable for engineering design with lower computing resources and costs [3].

The existing global reaction mechanism usually fixes the reaction order and the activation energy factor, limitedly suitable for specified thermodynamic parameters or reaction conditions. Thus, the computation accuracy has been questioned, applied the existing mechanisms in a wide range of reaction states. Marinov and Westbrook et al. [4] proposed a global reaction mechanism, which was applied to accurate prediction of laminar flame speed under the constant atmospheric pressure. It could show a very good approximation to the detailed mechanism with different equivalence ratios under the fixed initial temperature and pressure. The above mechanism determined the given pre-exponential factor and activation energy in Arrhenius equation, only considering the laminar flame propagation speed under the constant pressure. Furthermore, researchers developed the one-step global reaction under high temperature conditions [3,5–8], and they were well used in forecasting explosion problem under equivalence ratio conditions. Wang et al. [3] developed single-step chemistry model to predict the defloration to detonation process considering embedded obstacles in the plane channel, and obtained good numerical results. Kohany and Dahan [9] employed the one-step reaction mechanism to replace the detailed mechanism, and simulated the hydrogen combustion in jet flows utilizing the commercial software ANSYS. They hence assessed the effects of the one-step mechanism by the ability to predict the flammability limit of non-premixed gas mixture of hydrogen and oxygen [10,11].

Recently, a single-step reaction model developed by a calibration method was used in the work for stoichiometric hydrogen-air flames [12], which showed that the single-step chemical model was helpful in simulating flame dynamics and understanding the physics of hydrogen flames related on stabilities and propagation in confined tubes [13–16]. However, the establishment of the one-step global reaction mechanism is still very inadequate for fast and accurate predictions of ignition in practical problems, for instance supersonic combustion applied in the scramjets. Therefore, it is necessary for engineering application to develop a global reaction mechanism with higher accuracy and adaptability, which as well as can be coupled into the CFD solver to obtain accurate predictions of combustion.

On the other hand, researchers could use the detailed chemical reaction mechanism to predict the ignition delay time or the ignition position [17–22] in supersonic combustion. Moreover, most studies were conducted in the supersonic mixing layer flows or spatial jets. The mixing layer flow consists of the shear of two supersonic streams with different fluid and thermodynamic properties, to enhance the precombustion mixing between fuels and oxidizers. It is a very fundamental flow prototype occurred in scramjet combustors, and widely used to study the mixing and combustion physics in academia. Therefore, the supersonic chemically reacting mixing layer flows were also employed in this study.

In this paper, a one-step global reaction mechanism of hydrogen and air was developed based on the principle of obtaining a consistent and accurate ignition delay time compared with the detailed mechanisms. Different from the other one-step mechanisms, the database of activation energy factor was constructed under wider conditions of thermodynamic parameters. Coupled with the present reaction mechanism, the combustion in supersonic mixing layers was predicted and compared using an in-house CFD code to assess the present one-step mechanism of H_2/O_2.

Database construction of one-step mechanism

The detailed mechanism and ignition delay time

There are amount of reaction mechanisms of oxygen and hydrogen. For instance, a detailed mechanism including 10 species and 19 primitive reactions was given in Refs. [23–26], and some reduced mechanisms were presented in Refs. [27,28]. The detailed mechanism [29] is an update of previous one [24]. In this study, the detailed mechanism chosen from Ref. [23], as shown in Appendix A, because it was well validated and could accurately predict the H_2/O_2 reaction over a wide range of conditions even for the high-pressure regime. The reaction rates is generally denoted as,

$$K = AT^n \exp(-E/RT) \tag{1}$$

where n is the reaction order, E the activation energy factor. Thus, the selected mechanism spans pressure, temperature and residence time ranges of 0.3–15.7 atm, 850–1040 K, and 0.03–1.4 s, respectively. These data then span the explosion limit behavior of the system and place significant emphasis on HO_2 and H_2O_2 kinetics. The explosion limits of dilute $H_2/O_2/N_2$ mixtures extend to higher pressures and temperatures than those previously observed for undiluted H_2/O_2 mixtures.

The one-step reaction mechanism developed in this study will be based on the accurate prediction of ignition delay time. The ignition delay time (also called the induction time) is an important aspect to describe combustion characteristics. In this study it is taken as an important basic parameter for reducing the detailed reaction mechanism, At this instant, the reaction begins intensely and the mole numbers of intermediates or chain carriers such as O, H, OH, HO_2, for the reaction of H_2/O_2, increase by many orders of magnitude. A numerical method to determine the ignition delay time, τ , of a reacting system is defined as,

Please cite this article in press as: Wang B, et al., Construction of one-step H_2/O_2 reaction mechanism for predicting ignition and its application in simulation of supersonic combustion, International Journal of Hydrogen Energy (2016), http://dx.doi.org/10.1016/j.ijhydene.2016.09.010