

An evaluation of detailed reaction mechanisms for hydrogen combustion under gas turbine conditions

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Abstract

Chemical kinetics in hydrogen combustion for elevated pressures have recently become more relevant because of the implementation of hydrogen as a fuel in future gas turbine combustion applications, such as IGCC or IRCC systems. The aim of this study is to identify a reaction mechanism that accurately represents H_2/O_2 kinetics over a large range of conditions, particularly at elevated pressures as present in a gas turbine combustor. Based on a literature review, six mechanisms of different research groups have been selected for further comparisons within this study. Reactor calculations of ignition delay times show that the mechanisms of Li et al. and Ó Conaire et al. yield the best agreement with data from shock tube experiments at pressures up to 33 bar. The investigation of one-dimensional laminar hydrogen flames indicate that these two mechanisms also yield the best agreement with experimental data of laminar flame speed, particularly for elevated pressures. The present study suggests that the Li mechanism is best suited for the prediction of H_2/O_2 chemistry since it includes more up-to-date data for the range of interest.

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1. Introduction

One possibility to reduce CO_2 emissions from power production with fossil fuels is to convert the fuels to gas mixtures consisting mainly of hydrogen and carbon dioxide, and to separate CO_2 from the fuel prior to combustion in a gas turbine process, such as IGCC/IRCC systems. This necessitates the development of a gas turbine combustor for H_2 -rich fuels. Hydrogen has some characteristics that strongly deviate from the main components of conventional fuels, as e.g. methane. The hydrogen molecule is very light and therefore strongly exposed to molecular diffusion processes. Furthermore, hydrogen is a very reactive species with a large flammability range. These characteristics result in a high laminar flame speed of hydrogen/air mixtures. The relatively high adiabatic temperatures of H_2 /air mixtures might cause large amounts of thermal NO_x in the flame. The flame temperature, and therefore NO_x emissions, can be reduced by dilution with nitrogen or steam,

which lowers the efficiency of the process. A more advanced way for NO_x reduction is lean pre-mixing of fuel and air. However, the high reactivity and flame speed of pre-mixed H_2 /air mixtures enhances the danger of auto-ignition and flashback, respectively.

Detailed kinetic mechanisms are necessary to predict auto-ignition, flashback, and NO_x emissions. These mechanisms can also be used within CFD calculations to predict the turbulent reacting flow field inside a combustor. This study is solely dedicated to the reaction kinetics of hydrogen and air. Only pure H_2/O_2 kinetics are considered, i.e. N_2 is treated as inert and reactions for NO_x formation are neglected. Even though evaluation of NO_x was not a part of the present work, the authors emphasize the importance of the H_2/O_2 kinetics for accurate prediction of NO_x chemistry. The small amounts of hydrocarbons prevailing in a real fuel after a reforming process, are not accounted for. This strongly reduces the size of the reaction mechanism. While a typical mechanism for methane consists of around 50 species and 300 reactions, only eight species (without N_2) and about 20 reversible reactions are sufficient to describe pure H_2/O_2 kinetics.

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The aim of this study is to identify a reaction mechanism that accurately represents H_2/O_2 kinetics over a large range of conditions, particularly at elevated pressures between 15 and 35 atm as present in a typical gas turbine combustor. First, a review of reaction mechanisms for hydrogen combustion is given. Then, ignition delay times computed by some selected mechanisms using a closed homogeneous reactor model are compared to experimental data for a large range of pressures. Flame speeds of laminar premixed hydrogen flames are calculated with several mechanisms using a one-dimensional flame code and validated against measurements at atmospheric and elevated pressures. Finally, the results are discussed and concluding remarks are given.

2. Reaction mechanisms for hydrogen combustion

A large number of detailed mechanisms including H_2/O_2 kinetics can be found in the literature. Some of these mechanisms have been optimized for the combustion of pure hydrogen, but most of them are dedicated to the combustion of hydrocarbons including sub-mechanisms for H_2/O_2 chemistry. However, the accuracy of the H_2/O_2 subset is also essential for the overall performance of a hydrocarbon mechanism. In this study, only the mechanisms validated and used for hydrogen combustion are considered.

At the Gas Research Institute (GRI), the well-known GRI mechanism has been developed for C_1/C_2 kinetics [1,2]. The most recent version ‘GRI-Mech 3.0’ [3] contains 26 reversible reactions for H_2/O_2 kinetics. The GRI mechanism is optimized for natural gas combustion, but has also been validated against experimental data for ignition delay of stoichiometric hydrogen/air mixtures at 1 and 2 atm.

The research group around F.L. Dryer at Princeton University has been working on combustion kinetics for more than 20 years. In 1981, Westbrook and Dryer [4] gave a comprehensive review about chemical kinetics of combustion processes stating that the H_2/O_2 mechanism is well validated for a large number of application areas. However, much effort has been invested to optimize this mechanism later on, particularly for non-atmospheric pressures. A detailed hydrocarbon mechanism was published [5] including a H_2/O_2 subset of 21 reversible reactions. Yetter et al. [6] presented a detailed $CO/H_2/O_2$ mechanism containing 19 reversible reactions for the H_2/O_2 system that was validated against experimental data within a temperatures range of 823–2870 K, equivalence ratios between 0.0005 and 6.0, and pressures between 0.3 and 2.2 atm. This mechanism was further improved by Kim et al. [7] using experimental results of a flow reactor for pressures from 1 to 9.6 atm, temperatures from 960 to 1200 K, and equivalence ratios from 0.33 to 2.1. Mueller et al. [8] adjusted the H_2/O_2 system of this mechanism to experimental data over pressures and temperatures of 0.3–15.7 atm and 850–1040 K, respectively. Recently, Li et al. [9] updated the H_2/O_2 mechanism and validated it against a wide range of experimental conditions (298–3000 K, 0.3–87 atm, $\phi = 0.25 - 5.0$) found in laminar premixed flames, shock tubes, and flow reactors. The mechanism is named comprehensive due to excellent agreement of

the model predictions with an extensive set of experimental data.

Based on the mechanism of Mueller et al. [8], another so-called comprehensive H_2/O_2 mechanism with 19 reversible reactions has been developed by Ó Conaire et al. [10] at the National University of Ireland in Galway. The mechanism has been validated against experiments at temperatures ranging from 298 to 2700 K, pressures from 0.05 to 87 atm, and equivalence ratios from 0.2 to 6.

The research group around F.A. Williams at the University of California in San Diego developed a 21-step chemical scheme for hydrogen combustion [11]. This mechanism was recently extended to 22 reactions by Del Álamo et al. [12] and validated against experimental data of ignition delay at pressures up to 33 bar.

The research group around J. Warnatz has also strongly contributed to the development of combustion kinetics. In 1988, Maas and Warnatz [13] presented a detailed $CO/H_2/O_2$ mechanism for modeling of ignition processes. This mechanism was extended for C_1/C_2 species oxidation by Baulch et al. [14]. The H_2/O_2 subset of the mechanism in the latest textbook of Warnatz et al. [15] contains 19 reversible reactions. Through a personal communication, Warnatz [16] provided another H_2/O_2 mechanism that differs slightly from the one in his textbook. Preliminary, computations of ignition delay times have shown that this mechanism performs slightly better than the mechanism in his textbook.

Many other mechanisms have been referred to in the literature. Some of the most recent developments are an optimized kinetic model of H_2/CO combustion by Davis et al. [17] and a refined hydrogen combustion mechanism by Konnov [18]. The latter is based on the methane mechanism of Konnov [19] containing 28 reversible reactions for H_2/O_2 chemistry and has been validated against a large range of experimental data for hydrogen combustion. At Leeds University, a methane mechanism including a H_2/O_2 subset of 46 single reactions has been developed [20]. The H_2/O_2 mechanism of Marinov et al. [21] including 20 reversible reactions was validated against atmospheric laminar flame speed experiments, low-pressure laminar flame compositions, and ignition delay data at 2 atm. Katta and Roquemore [22] used a $H_2/O_2/N_2$ mechanism of Cowart et al. [23] with a H_2/O_2 subset of 17 reversible reactions for the simulation of a premixed H_2 /air Bunsen-type flame. They yielded good agreement of predicted and measured burning velocities at different equivalence ratios at atmospheric pressure. Cain [24] used a mechanism of Jachimovski and Mclain [25] containing 17 reversible reactions for the simulation of auto-ignition of hydrogen at pressures between 3.5 and 7 MPa. Miller and Bowman [26] developed a detailed mechanism for nitrogen chemistry including 20 reversible reactions for H_2/O_2 kinetics. Glarborg et al. [27] constructed a mechanism for hydrocarbon/nitric oxide interactions with 22 reversible reactions for H_2/O_2 kinetics. Lindstedt et al. [28] developed a mechanism for ammonia oxidation based on the H_2/O_2 kinetics of Baulch et al. [14].

Furthermore, some comparative studies of various mechanisms have been performed. Qin et al. [29] compared predicted

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