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The effect of temperature on the adiabatic burning velocities of diluted hydrogen flames: A kinetic study using an updated mechanism

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ABSTRACT

The effect of temperature on the adiabatic burning velocities of diluted hydrogen flames has been analyzed using an updated version of the Konnov detailed reaction mechanism for hydrogen. The contemporary choice of the reaction rate constants is provided with the emphasis on their uncertainties, and the analysis of the performance of the updated mechanism is presented and compared to the previous version for a wide range of validation cases: jet stirred and flow reactors; oxidation, decomposition and ignition in shock waves; ignition in rapid compression machines; laminar burning velocity and flame structure. An overall improvement of the mechanism performance was observed, particularly for the shock tube and flow reactor studies. Temperature dependence of the burning velocity, S_L, is commonly interpreted using the correlation $S_L = S_{L0}(T/T_0)^{\alpha}$. The updated mechanism was applied to study the behavior of the power exponent α for $H_2 + O_2 + N_2$ flames in a wide range of stoichiometry and dilution ratios. The simulations were compared to the available experimental results, either taken from the literature or evaluated in the present study from the existing burning velocity data. The equivalence ratio and N_2 content in the mixture were found to have significant influence on the temperature power exponent. The dependence of the temperature exponent on the fitting temperature range was observed and discussed. This effect was found to cause significant discrepancies in the burning velocities at high temperatures, if obtained with empirical correlation.

1. Introduction

Hydrogen-fueled internal combustion engines and stationary gas turbines in integrated gasification combined cycle (IGCC) technology burning high hydrogen content syngas mixtures are nowadays the most realistic and promising examples of hydrogen-based economy. Further development and optimization of these technologies requires detailed knowledge of combustion characteristics of hydrogen at elevated pressures and temperatures. The laminar burning velocity is one of these characteristics that defines the rate of fuel consumption in laminar flames, and also relates to blow-off and flash-back phenomena. Moreover, contemporary models of turbulent flame propagation are calibrated by the laminar burning velocity at specific (local) conditions of composition, temperature, pressure, and dilution by products. Since the laminar burning velocity depends on the limited number of these parameters it can be described by mathematically simple correlations valid over the desired range of conditions.

Very often the effects of composition, temperature, pressure, and dilution by products are considered to be independent. For instance, the correlation describing the influence of initial temperature on the adiabatic laminar burning velocity and used in this or equivalent form since 1950s, e.g., [1],

$$S_L = S_{L0}(T/T_0)^{\alpha} \tag{1}$$

includes the reference temperature, T_0, and the burning velocity at this temperature, S_{L0}, varying with equivalence ratio, ϕ. Pressure dependence of the power exponent coefficient, α, in Eq. (1) was often neglected or averaged. Earlier measurements of the power exponent α for hydrogen + air flames [1–4] at pressures around 1 atm were summarized by Konnov [5]. These experimental results have been compared with the power exponents derived from the modeling employing detailed reaction mechanism for hydrogen combustion [6]. Satisfactory agreement was found with the results of Heimel [1] and with the correlations of Liu and MacFarlane [2] and of Iijima and Takeno [4] from stoichiometric to moderately rich ($\phi = 3$) mixtures. In the lean and very rich mixtures, however, the

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calculated power exponent increases dramatically and significantly deviates from the linear type correlations [2,4]. Discrete measurements of Verhelst et al. [7] in lean hydrogen flames at atmospheric pressure showed large scattering as can be seen in Fig. 1. Hu et al. [8] performed limited set of experiments at elevated temperatures and supported their measurements by the modeling employing the mechanism of Ó Conaire et al. [9]. For stoichiometric hydrogen + air flames at 1 atm they found that the calculated power exponent α increases with the temperature increase from 300 to 900 K and described this variation as $\alpha = 1.319 + 8.019 \cdot 10^{-4} \cdot T$, which gives the value of 1.56 at 300 K also shown in Fig. 1. Recent experimental study of Gerke et al. [10] covered a range of temperatures from 350 to 700 K and pressures from 5 to 45 atm. The authors derived empirical correlation for the pressures above 10 atm and equivalence ratios $0.4 < \phi < 2.5$ as $\alpha = 0.0163/\phi + 2.2937$. This expression is not shown in Fig. 1 since, as will be discussed below, the power exponents do depend on the pressures. Similar to the work of Hu et al. [8], Gerke et al. [10] implemented the mechanism of Ó Conaire et al. [9] and derived a correlation covering extended range of pressures ($1 < P < 80$ atm); the calculated power exponents from both studies are also depicted in Fig. 1. Contrary to the finding of Hu et al. [8] their correlation for α does not depend on temperature.

Rakopoulos et al. [11] compared correlations derived from experiments available in the literature and found that they are significantly different at conditions relevant to hydrogen-fueled engines, i.e., they predict laminar burning velocities diverged by a factor of two. Further experiments on hydrogen flame propagation are therefore highly desired. Meanwhile several groups derived burning velocity correlations thanks to the availability of detailed kinetic models for hydrogen combustion. D'Errico et al. [12] employed the reaction scheme developed by Frassoldati et al. [13] and calculated burning velocities of lean hydrogen + air flames from atmospheric pressure up to 16 atm. Bougrine et al. [14] attempted several models and selected GRI-mech 3.0 [15] for the modeling of methane + hydrogen flames in the full range of fuel compositions up to 100% of H_2. Verhelst and Sierens [16] chose the mechanism of Yetter et al. [17] for S_L correlation at 1–16 atm., and in the later study of Verhelst et al. [18] the model developed by Konnov [6] was used in the pressure range of 5–45 atm. Szabo et al. [19] selected rather old mechanism of Maas and Warnatz [20] integrated into the code INSFLA. The study of Ravi and Petersen [21] was motivated by the recent appearance of an updated detailed kinetic model for hydrogen and syngas combustion [22]. They clearly demonstrated that the power exponents α increase with the pressure increase and discussed different approaches of simultaneous description of the burning velocity variation with temperature and pressure. Thus, for the fair comparison, in Fig. 1 the power exponents α from these works [8,10,12,14,16,18,21] are shown if they were computed at 1 atm. Kusharin et al. [23] studied expanding spherical flames experimentally and numerically, and their value of α from the modeling with the mechanism of Warnatz [24] for H_2 + air mixture is also shown in Fig. 1.

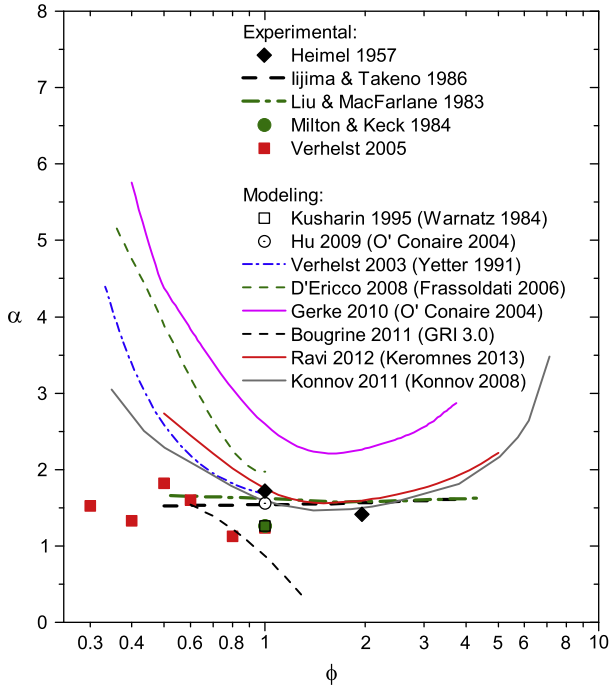

Fig. 1. Power exponent α for hydrogen + air flames at conditions close to atmospheric pressure and 298 K. Solid symbols and thick lines: experiments [1–4,7], open symbols and thin lines: modeling and correlations [5,8,10,12,14,16,21,23]. For the modeling studies, the implemented kinetic mechanisms [6,9,13,15,17,22,24] are given in the parentheses in the legend.

The influence of diluents added into combustible mixture on the burning velocity is considered to be independent from the temperature dependence with typical linear correlation term:

$$S_L = S_{L0}(T/T_0)^{\alpha}(1 - F(\phi, T_0, \text{diluent}) * f) \quad (2)$$

where dilution ratio f is defined as the volume of the diluent divided by the total volume of the mixture (diluent + air + fuel). The coefficient of proportionality F representing the slope of corresponding dependences is known to be different for different diluents, e.g., [25,26]. It is now well established that it also depends on the initial temperature and stoichiometric ratio, e.g., [27,28].

The variation of the power exponents α with increased amount of steam or nitrogen added to stoichiometric hydrogen flames has been first studied by Kusharin et al. [23] at pressures around 1.5 atm. They observed that increased amount of diluent makes the flames more sensitive to the initial temperature of the mixture and thus the power exponent increases. This finding is consistent with the work of Zitoun and Deshaies [29] who investigated hydrogen + oxygen (no diluent) flames and for stoichiometric mixture found $\alpha = 0.9$, the value which is much lower than those shown in Fig. 1 for H_2 + air flames. Zitoun and Deshaies [29] also admitted that their burning velocity measurements are systematically 20% higher than earlier results of Edse and Lawrence [30], yet noted good agreement in terms of the temperature dependence. Increase of the power exponent coefficient α with dilution by nitrogen has been also observed by Vancoillie et al. [28] in methanol + oxygen + nitrogen mixtures.

Most recently Paidi et al. [31] performed a dedicated study of the effect of dilution by N_2 or CO_2 on the laminar burning velocity of hydrogen flames at elevated temperatures up to 600 K. Two dilution ratios defined as the diluent volume over the volume of (diluent + fuel) in the mixtures were studied. It was demonstrated that the power exponent coefficients α increase at higher dilution ratio. These experiments were found in satisfactory agreement with the modeling performed using the mechanism of Li et al. [32]. Experimentally obtained coefficients α, however, progressively deviate from the calculated values in rich mixtures [31].

There are two apparent reasons for significant differences in the power exponent coefficients α predicted by different detailed kinetic schemes as seen in Fig. 1. First, the modeling has been performed over different ranges of pressures and temperatures that affect pressure-dependent coefficients α as mentioned above. Moreover, in the correlation studies, the validation domain is centered at the engine-like conditions, so that if a single expression for α was obtained for the whole pressure range, it can be expected to