Sub-atmospheric flame speeds: Interest and difficulty to improve kinetic modeling

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Description of hydrogen combustion is important for at least two reasons: hydrogen is a renewable fuel, biologically or chemically derived, which burns intensely and cleanly and its oxidation mechanism forms the basic building block required in oxidation mechanisms of more complex fuels. Extensive research has been conducted experimentally and numerically on the reactivity of hydrogen/air or hydrogen/oxygen mixtures, including diluted mixtures and high pressure conditions. Although the combustion of hydrogen under standard conditions is globally well simulated, the effect of pressure and equivalence ratio variations is less accurately captured. Furthermore, whereas recent efforts concerned high-pressure flames, only few data have been obtained under reduced pressure where non-monotonic variation of flame speed with pressure has been reported. The sub-atmospheric conditions, and more specifically around 200 mbar, are of particular importance to guarantee a safe operation of the International Thermonuclear Experimental Reactor (ITER). Updates of hydrogen kinetic reaction mechanism have been recently presented and are tested against the present experimental data. Though mainly focused on high pressures, the mechanisms of Burke et al. [1] and Keromnès et al. [2] were selected in the current study. Experimental measurements of laminar flame speed, analysis of the key reactions and kinetic pathways, and modeling studies were performed for H_2-air premixed flames over a wide range of conditions: equivalence ratios ranged from 0.5 to 4.0 and pressures from 0.2 to 3 bar.

Laminar flame burning velocity measurements were performed using a stainless steel spherical combustion chamber with an inside volume of 4.2 L used previously. The chamber was filled with synthetic air and pure hydrogen. The composition of synthetic air was: 20.9%vol of O_2 and 79.1%vol of N_2. Air and hydrogen were injected using thermal mass flow meters. The temperature of the chamber was regulated at T_u = 303 K. Inside the chamber, an electric fan mixed the reactants. Two tungsten electrodes separated by 1 mm, connected to a capacitive discharge ignition system, were used for spark ignition at the chamber center. In all experiments, the inside chamber total pressure can be considered as constant. Shadowgraphy was used to record flame images. Computations were performed using the CHEMKIN package and the PREMIX code. We compared our experimental results obtained at four different equivalence ratios (0.5, 1, 1.7, and 3) as a function of the pressure to the laminar burning velocities calculated with both of these kinetic mechanisms (Figure1).

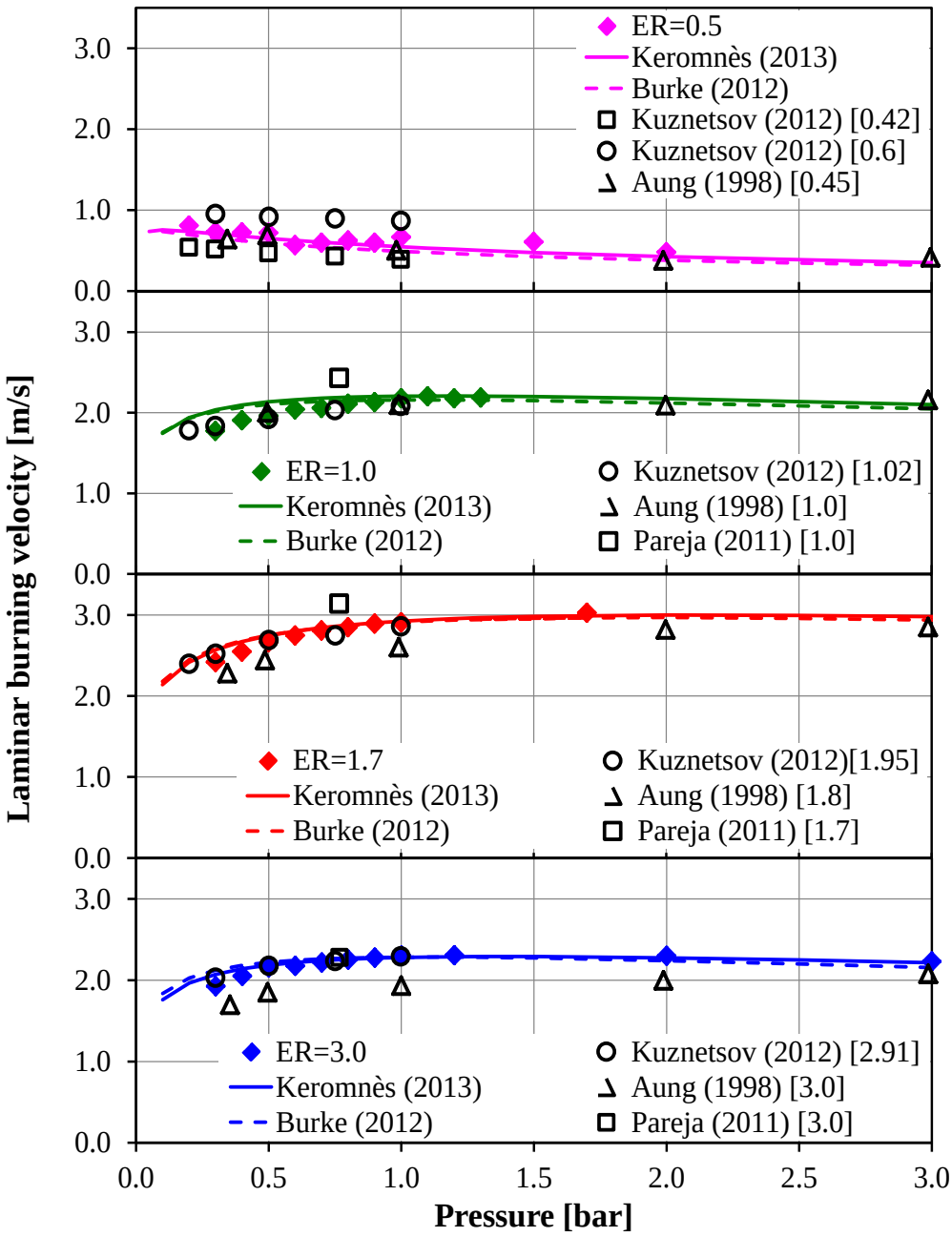

Figure 1. Laminar burning velocity of hydrogen/air mixtures according to the initial pressure at T_u = 303 K and (a) φ = 0.5, (b) φ = 1.0, (c) φ = 1.7, and (d) φ = 3.0. Symbols are experimental results, lines are calculations (equivalence ratios are given in parentheses).

[1] M.P. Burke, M. Chaos, Y. Ju, F.L. Dryer, S.J. Klippenstein, Int. J. Chem. Kinet. 44 (2012) 444-474.

[2] A. Keromnes, W.K. Metcalfe, K.A. Heufer, N. Donohoe, A.K. Das, C.J. Sung, J. Herzler, C. Naumann, P. Griebel, O. Mathieu, M.C. Krejci, E.L. Petersen, W.J. Pitz, H.J. Curran, Combust. Flame 160 (2013) 995-1011.