Study of the flame structure of CH_4/H_2 mixtures at elevated pressure and development of reduced reaction mechanism

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Understanding and controlling the combustion of clean and efficient fuel blends, like methane + hydrogen, is essential for optimizing energy production processes and minimizing environmental impacts. To extend the available experimental database on CH_4+H_2 flame speciation, the novel measurement data for chemical speciation and thermal structure of laminar premixed burner-stabilized $CH_4/H_2/O_2/Ar$ flames at different equivalence ratios (φ=0.8 and φ=1.2), hydrogen contents in the CH_4/H_2 blend (X_{H2}=25%, 50% and 75%) and pressures (1, 3 and 5 atm) was obtained. The flame-sampling molecular-beam mass spectrometry (MBMS) technique was used to detect reactants, major products, and several combustion intermediates, including major flame radicals. The mole fraction profiles of the some key intermediates (H, OH, CH_3, HO_2, H_2O_2, formaldehyde, acetylene, ethylene and ethane) were measured. The experimental data presented in this work extend the available experimental database for the chemical speciation of flames fueled by CH_4/H_2 mixtures at elevated pressures and can be used for the validation of relevant chemical kinetic models.

The experimental profiles of the species mole fractions were utilized to validate the detailed chemical kinetic mechanism AramcoMech 2.0 and reduced kinetic mechanisms RMech1 (30 species and 70 reactions) was developed employing a combination of several methods (DRG, ROP and CSP) and using ignition delays, maximum temperature and concentrations of important intermediates as targets. The even compact kinetic mechanism RMech2 (21 species and 31 reactions) was obtained starting with RMech1 and using ROP and sensitivity analyses. Both mechanisms were demonstrated to reasonably capture numerous literature data for the laminar burning velocity values and ignition delays of methane/hydrogen fuel blends, and demonstrated a good predictive ability of the structure of fuel-lean flames (φ=0.8), which is close to the desirable gas-turbine conditions. This suggests that these mechanisms have good prospects to be used for the CFD calculations of processes in realistic combustion devices.

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