Hydrogen oxidation at high pressure and intermediate temperatures: experiments and kinetic modeling - DTU Orbit (14/03/2019)

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Hydrogen oxidation at 50 bar and temperatures of 700–900 K was investigated in a high pressure laminar flow reactor under highly diluted conditions. The experiments provided information about H₂ oxidation at pressures above the third explosion limit. The fuel–air equivalence ratio of the reactants was varied from very oxidizing to strongly reducing conditions. The results supplement high-pressure data from RCM (900–1100 K) and shock tubes (900–2200 K). At the reducing conditions (U = 12), oxidation started at 748–775 K while it was shifted to 798–823 K for stoichiometric and oxidizing conditions (U = 1.03 and 0.05). At very oxidizing conditions (O₂ atmosphere, U = 0.0009), the temperature for onset of reaction was reduced to 775–798 K. The data were interpreted in terms of a detailed chemical kinetic model, drawn mostly from work of Burke and coworkers. In the present study, the rate constants for the reactions HO₂ + OH, OH + OH, and HO₂ + HO₂ were updated based on recent determinations. The modeling predictions were in good agreement with the measurements in the flow reactor. The predicted H₂ oxidation rate was sensitive to the rate of the HO₂ + OH reaction, particularly at lean conditions, and the present data support recent values for the rate constant. In addition to the current experiments, the mechanism was evaluated against ignition delay time measurements from rapid compression machines and shock tubes. The model was used to analyze the complex dependence of the ignition delay for H₂ on temperature and pressure.