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Abstract

A series of experimental and numerical investigations into hydrogen oxidation at high pressures and intermediate temperatures has been conducted. The experiments were carried out in a high pressure laminar flow reactor at 50 bar pressure and a temperature range of 600–900 K. The equivalence ratio of the mixture was varied from oxidizing to reducing conditions. Moreover, a series of experiments in an oxygen atmosphere instead of a nitrogen atmosphere has been done. A reaction mechanism based on a recent work by Burke et al. has been developed. In addition to modeling of the present experiments, the mechanism is used to simulate published data on ignition delay time and laminar burning velocity of hydrogen. The flow reactor results show that at reducing, stoichiometric, and oxidizing conditions, conversion starts at temperatures of 750–775 K, 800–825 K, and 800–825 K, respectively. In oxygen atmosphere, ignition occurs at the temperature of 775–800 K. In general, the present model provides a good agreement with the measurements in the flow reactor and with recent data on laminar burning velocity and ignition delay time.

Experimental Setup – Laminar Flow Reactor

- Quartz reactor to minimize surface reactions
- Steel pressure shell to achieve high pressures
- Temperature: 600–900 K
- Pressure: 50 bar
- Flow: 3.06 NLM/min
- Isothermal Zone Length: 42–44 cm
- Residence time: 6.3–8.0 s
- Measurement via a GC and a Gas Analyser

Results (The Flow Reactor)

- Reaction Kinetics Model
  - Developed based on the mechanism by Burke et al. [1]
  - Updated rates for reactions of
    \[ \text{OH} + \text{OH} = \text{O} + \text{H}_2\text{O}, \]
    \[ \text{HO}_2 + \text{OH} = \text{H}_2\text{O}_2, \]
    \[ \text{HO}_2 + \text{H}_2 = \text{H}_2\text{O}_2 + \text{O}. \]
- Solution via Chemkin-Pro

Results (Comparison to Available Data)

- Results of stoichiometric experiments (0.95% H₂ and 0.04% O₂ in N₂, φ=1.20) at 50 bar pressure.
- Results of reducing experiments (0.95% H₂ and 0.04% O₂ in N₂, φ=1.20) at 50 bar pressure.
- Results of oxidizing experiments (0.18% H₂ and 1.60% O₂ in N₂, φ=0.05) at 50 bar pressure.

Summary

The flow reactor results show that at reducing, stoichiometric, and oxidizing conditions, conversion starts at temperatures above 750 K, 900 K, and 800 K, respectively. In oxygen atmosphere, ignition occurs at temperatures above 775 K. The changes in the model improve its prediction especially at oxidizing conditions. Ignition delay time of hydrogen shows a non-linear trend versus pressure especially at low temperatures. The present chemical scheme used in a constant u & v model is able to predict the trend reasonably well while for a more accurate prediction at low temperatures, it is required to consider device-dependent pressure (and temperature) rise before the ignition. Predictions of laminar burning velocity by the model are within the uncertainty of the experiments. In general, the present model provides a better agreement to the measurements comparing to the base model.

References