

## A Detailed Chemical Kinetic Model for Syngas Combustion at Elevated Pressure

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A detailed chemical kinetic mechanism for hydrogen and H<sub>2</sub>/CO (syngas) mixtures has been developed to reflect new experimental information obtained at high pressures, and new rate constant values recently published in the literature. In the mechanism validation, particular emphasis is placed on reproducing behavior at high pressures and intermediate to high temperature conditions which are important for applications in internal combustion engines and gas turbines. The mechanism has been validated over a wide range of conditions: at pressures of 1 to 70 atmospheres, at temperatures in the range of 900–2500 K and equivalence ratios from 0.1 to 5.0 using diluent gases based on nitrogen, argon and helium. The detailed chemical kinetic model agrees well with ignition delay times up to 70 bar and with laminar flame speeds from 1 to 40 atmospheres. The reaction sequence H<sub>2</sub> + HO<sub>2</sub> = H + H<sub>2</sub>O<sub>2</sub> followed by H<sub>2</sub>O<sub>2</sub> (+M) = OH + OH (+M) was found to play a key role in hydrogen ignition under high-pressure and intermediate-temperature conditions. The rate constant for H<sub>2</sub> + HO<sub>2</sub> showed strong sensitivity for high-pressure ignition times and has considerable uncertainty based on literature values. A rate constant for this reaction is recommended based on available literature values and our mechanism validation.

Syngas mixture oxidation was investigated experimentally and simulated with the revised chemical kinetic model. Ignition delay times for H<sub>2</sub>/CO/O<sub>2</sub>/N<sub>2</sub>/Ar mixtures have been measured inside rapid compression machine (RCM) and shock tubes at pressures from 1 to 70 bar, for a temperature range of 900–2550 K and equivalence ratio from 0.1 to 4.0. Results show a strong dependence of the ignition delays to compressed temperature and pressure. Ignition delays decrease with increasing temperature, pressure and equivalence ratio. The reactivity of the syngas mixtures is governed by hydrogen chemistry for CO concentration lower than 50% in the fuel mixture. For higher CO concentrations, an inhibiting effect of CO was measured. Experimental results have been compared to our newly revised chemical kinetic mechanism and show good agreement.