Experimental and Kinetic Modeling Study of Methanol Ignition and Oxidation at High Pressure - DTU Orbit (30/04/2019)

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A detailed chemical kinetic model for oxidation of CH3OH at high pressure and intermediate temperatures has been developed and validated experimentally. Ab initio calculations and Rice–Ramsperger–Kassel–Marcus/transition state theory (RRKM/TST) analysis were used to obtain rate coefficients for CH2OH ⇌ CH2O+H, CH3O⇌ CH2O+H, CH3O⇌ CH2 OH , and CH 3O+O2⇌ CH 2O+ HO 2. The experiments, involving CH3OH/O2 mixtures diluted in N2, were carried out in a high-pressure flow reactor at 600–900 K and 20–100 bar, varying the reaction stoichiometry from very lean to fuel-rich conditions. Under the conditions studied, the onset temperature for methanol oxidation was not dependent on the stoichiometry, whereas increasing pressure shifted the ignition temperature toward lower values. Model predictions of the present experimental results, as well as rapid compression machine data from the literature, were generally satisfactory. The governing reaction pathways have been outlined based on calculations with the kinetic model. Unlike what has been observed for unsaturated hydrocarbons, the oxidation pathways for CH3OH under the investigated conditions were very similar to those prevailing at higher temperatures and lower pressures. At the high pressures, the modeling predictions for onset of reaction were particularly sensitive to the CH 3 OH + HO 2⇌ CH 2 OH +H2O2reaction.