Experimental and Modeling Investigation of the Effect of H2S Addition to Methane on the Ignition and Oxidation at High Pressures - DTU Orbit (03/04/2019)

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The autoignition and oxidation behavior of CH4/H2S mixtures has been studied experimentally in a rapid compression machine (RCM) and a high-pressure flow reactor. The RCM measurements show that the addition of 1% H2S to methane reduces the autoignition delay time by a factor of 2 at pressures ranging from 30 to 80 bar and temperatures from 930 to 1050 K. The flow reactor experiments performed at 50 bar show that, for stoichiometric conditions, a large fraction of H2S is already consumed at 600 K, while temperatures above 750 K are needed to oxidize 10% methane. A detailed chemical kinetic model has been established, describing the oxidation of CH4 and H2S as well as the formation and consumption of organo sulfuric species. Computations with the model show good agreement with the ignition measurements, provided that reactions of H2S and SH with peroxides (HO2 and CH3OO) are constrained. A comparison of the flow reactor data to modeling predictions shows satisfactory agreement under stoichiometric conditions, while at very reducing conditions, the model underestimates the consumption of both H2S and CH4. Similar to the RCM experiments, the presence of H2S is predicted to promote oxidation of methane. Analysis of the calculations indicates a significant interaction between the oxidation chemistry of H2S and CH4, but this chemistry is not well understood at present. More work is desirable on the reactions of H2S and SH with peroxides (HO2 and CH3OO) and the formation and consumption of organosulfuric compounds.

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