

Experimental study of the low- and high-temperature oxidation of dimethyl ether in a jet-stirred reactor

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Due to the current issue concerning the growing primary energy demand, not to mention a general interest in sustainable development, bio-fuels became very fashionable in recent years. They are subject to a lot of research on combustion with the characterization of the reactivity and pollutant emissions. The molecule of dimethyl ether (DME) has led to a strong interest in the field of combustion. Corresponding to the simplest linear ether ($\text{CH}_3\text{-O-CH}_3$), it has a high cetane value (55-60) and a low toxicity. Promising studies have highlighted key-strengths of this molecule as an additive agent or even an alternative diesel fuel. Among these advantages, we find a particularly significant decrease in the formation of soot and NO_x particles.

Due to its simplicity, DME is a good choice for understanding the mechanisms of ether oxidation. It exhibits typical "two-stages" ignition characteristics common to many hydrocarbons: low temperature, negative temperature coefficient, and hot ignition phenomena. Several experimental and theoretical studies have investigated on DME combustion, using various equipments (jet-stirred reactor, shock-tube, counterflow diffusion flame, variable-pressure flow reactor...) and at different operational conditions. Even if they bring essential information, they are unable to predict a single valid model for all circumstances. The objective of this study is to investigate DME oxidation with a different approach in order to complete existing experimental data, and subsequently better understand its reaction mechanism.

This was done with several experiments carried out in a jet-stirred reactor operating at 800 Torr, 500-1100 K, and at different equivalence ratios: 0.25, 1 and 2. The products obtained have been analyzed using two complementary methods: gas chromatography (GC) and cavity ring-down spectroscopy (CRDS). GC is efficient in separating compounds and allows us to analyse a wide range of products like CO, CO_2 , hydrocarbons, CH_3CHO and CH_3OCHO ; while CRDS is an absorption spectroscopic technique and allows us to analyze species such as CH_2O , H_2O and H_2O_2 (undetectable by GC).

Profiles of DME conversion and products were compared with expected theoretical profiles (cf. Zhao et al., J. of Chem. Kin. 2008,401-18). While they are quite similar at high temperatures, a significant difference appears at low temperature (from 500 to 750K). Whatever equivalence ratio studied, the model overestimates the conversion of the reactant over this range of temperature. Pre-established mechanisms are then not yet optimal and should be improved to better predict the oxidation of DME.

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