EXPERIMENTAL KINETICS STUDY IN LOW-PRESSURE LAMINAR FLAMES OF OME_1 AND OME_2

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The emergency of reducing the emission of greenhouse gases and achieving a circular carbon economy has encouraged research on renewable energy systems. For long-distance transportation and long-term storage, electricity can be converted into liquid and gaseous fuels (called e-fuels) benefiting from their high energy density. Oxymethylene ethers (OME_s) are regarded as one of the valuable candidates for e-fuels and potential asset to the current energy transition. A detailed knowledge of the chemical kinetics of OME_s is necessary to optimize their combustion properties. Moreover, few detailed studies have been conducted on longer chain species (OME_n, n>1) [1-3]. The purpose of this work is to refine the kinetics of OME_1 and to study the combustion chemistry of OME_2 in laminar low-pressure flames, under stoichiometric conditions, by carrying out experimental studies with molecular-beam mass spectrometry (MBMS) and kinetic modeling studies. A new detailed kinetic mechanism including OME_1 and OME_2 will be established and validated against these experimental flame structures.

Experimental methods, modeling, and results

A stoichiometric OME_1/oxygen/argon flame was stabilized at 50 mbar on a mobile Spalding-Botha burner. Species and radicals were measured and identified with MBMS for acquiring the structure of the neat OME_1 flame. The ionization potentials were measured and adjusted for each species to decrease the interferences either from fragmentation or from the overlapping of species with similar molecular masses. The structure of stoichiometric OME_2/oxygen/argon flame will be studied in the same experimental setup. The mechanism from Kathrotia et al. [3], which includes ethers from OME_0 to OME_5, was used for comparison with the OME_1 flame and will be used for the comparison with the OME_2 flame. The simulations with the mechanism are performed using OpenSMOKE++ [4].

Initial experimental results from the OME_1 flame show good agreement of the main species and intermediates, such as CO, H_2, C_2H_2, CH_4, CO_2, etc., with the results of the model. With the measurements of the OME_2 flame, the main oxidation routes of OME_1 and OME_2 will be determined and compared. The effects of chain length on the reaction pathway will be interpreted by comparing the consumption of the fuels and the formation of intermediate chemical species as well as radicals in both the OME_1 and OME_2 flames.

References

[1] He T, Wang Z, You X, Liu H, Wang Y, Li X, et al. "A chemical kinetic mechanism for the low- and intermediate-temperature combustion of Polyoxymethylene Dimethyl Ether 3 (PODE3) ", *Fuel*. 212:223–35 (2018)

[2] Cai L, Jacobs S, Langer R, vom Lehn F, Heufer KA, Pitsch H. "Auto-ignition of oxymethylene ethers (OMEn, n = 2–4) as promising synthetic e-fuels from renewable electricity: shock tube experiments and automatic mechanism generation", *Fuel.* 264:116711 (2020)

[3] Kathrotia T, Oßwald P, Naumann C, Richter S, Köhler M. "Combustion kinetics of alternative jet fuels, Part-II: Reaction model for fuel surrogate", *Fuel.* 302:120736 (2021)

[4] Cuoci A, Frassoldati A, Faravelli T, Ranzi E. "OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms", *Computer Physics Communications*. 192:237–264 (2015)

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Laminar flames