Kinetic characterization of OME_{1-3} oxidation using low-pressure laminar flames and shock tube measurements

Yanan Huo, Véronique Dias, Hervé Jeanmart

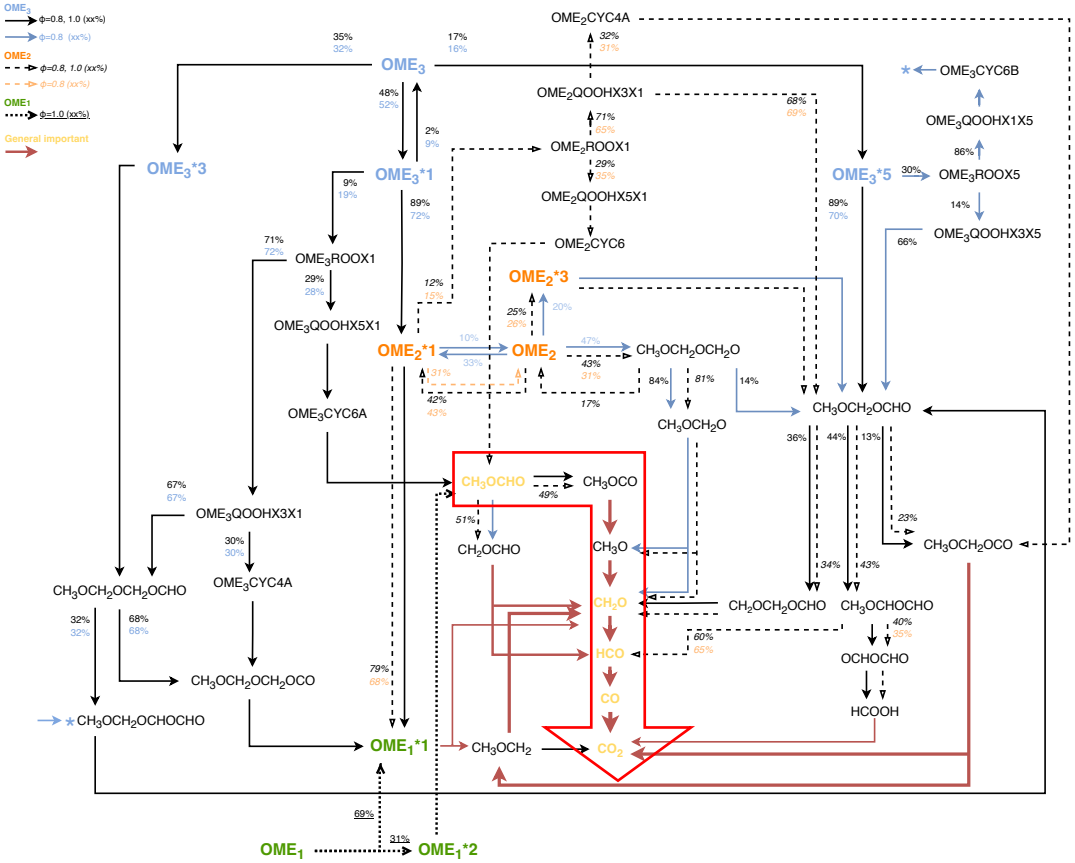
Institute of Mechanics, Materials and Civil Engineering (iMMC)
Université catholique de Louvain, Louvain-la-Neuve, Belgium
veronique.dias@uclouvain.be

The urgency of reducing greenhouse gas emissions and achieving a circular carbon economy has motivated research on renewable energy. For long-distance transportation and extended storage, electricity can be converted into liquid and gaseous fuels, referred to as e-fuel, benefiting from their high energy density. Oxymethylene ethers (OMEs) are considered a promising component in the ongoing energy transition and one of the significant candidates for e-fuels.

This work aims first to study the chemistry of low-pressure combustion of OME_2 and OME_3 in premixed laminar flames under equivalence ratio conditions of 0.8 and 1.0, by conducting experimental studies with MBMS and kinetic modeling. Next, a high-pressure study in a shock tube is used to measure the ignition delay times of OME_1 and OME_2 combustion under conditions of 0.5, 1.0, and 2.0, in a temperature range between 980 and 1350 K at a pressure of 20 and 40 bar.

The stoichiometric and fuel-lean neat OME_2 and OME_3 flames were stabilized at 50 mbar on a mobile Spalding-Botha burner. Species and radicals were measured and identified with MBMS to determine the flames' structure. The temperature profiles of both flames have been measured for the purpose of the kinetic modelling. The mechanism from Kathrotia et al. [1], has been used for comparison with the experimental results of the OME_2 and OME_3 flames. Based on these comparisons, the UCL mechanism [2] has been extended by analogy with OME_2 and OME_3 kinetics from other works.
The numerical modeling has been performed by using OpenSMOKE++. The experimental results from the OME_2 and OME_3 flames show good agreement for the main species and some intermediates. With the measurements of the flames and interpretation from the new UCL mechanisms, the dominant consumption pathways of OME_2 and OME_3 flames are determined, showing that the OME_1 chemistry is found to be crucial for the consumption pathways of OME_2 and OME_3 flames. The effects of chain length on the reaction pathways of two fuels are elucidated by comparing the formation of intermediates and the consumption pathway of the fuels.

At high pressure (20–40 bar), ignition delay time measurements and simulations provided complementary insight into the oxidation chemistry of OMEs under conditions dominated by pressure-dependent stabilization and peroxy radical pathways. The UCL model successfully reproduced the experimentally observed Arrhenius-type dependence of ignition delay times on temperature, as well as the systematic acceleration of ignition at higher pressures and for longer OMEs chain lengths.



Consumption pathway predicted by new UCL model for both OME_2 flames and OME_3 flames both under fuel-lean (Φ = 0.8) and stoichiometric (Φ = 1.0) conditions

References

[1] T. Kathrotia, P. Oßwald, J. Zinsmeister, T. Methling, and M. Kohler, Fuel 302, 120737 (2021)
[2] V. Dias, X. Lories, and J. V andooren, Combustion Science and Technology 182, 350 (2010)