EXPERIMENTAL AND NUMERICAL KINETIC STUDY OF OME_1 AND OME_2 COMBUSTION IN LOW-PRESSURE LAMINAR FLAME AND SHOCK-TUBE

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Introduction

The urgency of reducing the emission of greenhouse gases and achieving a circular carbon economy encourages research on renewable energy systems. The alternative synthetic fuels (power to liquids) could be high-potential energy carriers for long-distance transportation and long-term storage [1, 2]. Oxymethylene ethers (OME_s), formally known as polyoxyethylene dimethyl ethers, with the structural formula of $CH_3O(CH_2O)_nCH_3$, are regarded as a potential asset for the energy transition and valuable candidates for power to liquids thanks to their high energy density [3, 4]. A deep understanding of oxidation kinetics of OME_s remains a prerequisite for optimizing their combustion and for a comprehensive assessment of the future engine application potential of OME_s. Few detailed studies have been conducted on longer-chain OMEs (OME_n, n>1) [5-8]. The purpose of this work is to investigate the combustion chemistry of OME_1 and OME_2 under stoichiometric and fuel-lean conditions and develop a detailed mechanism including OME_{1-2}. The experimental study of OME_1 and OME_2 combustion was performed in the shock tube at high pressures and in laminar flames at low pressure by carrying out flame structure measurements with molecular-beam mass spectrometry (MBMS).

Experimental methods and numerical modeling

In the measurement of laminar flames under the stoichiometric and fuel-lean conditions, OME_1 and OME_2 flames were stabilized at 50 mbar on a mobile Spalding-Botha burner with a diameter of 8 cm. Parallel to the burner surface, a quartz cone (0.08 mm orifice) allows direct sampling from the flame with a distance range of 0-30 mm. Samples are measured with MBMS for which the ionization potentials were measured and adjusted for each species to decrease the interferences from fragmentation or overlapping species with similar molecular masses. The experimental flame temperature profiles will be measured in a next step.

The investigation of ignition delay times for mixtures of OME_1 and OME_2 was conducted within a high-pressure shock tube facility under the temperature range of 980 to 1350 K, at pressures of 20 and 40 bar with equivalence ratios of 0.5, 1, and 2. The stainless-steel shock tube, measuring 50 mm in diameter, is divided into a 4 m driver section and a 5 m driven section by a pair of stainless-steel diaphragms. Ignition delay times were determined by analyzing the pressure profiles captured by PCB 113B22 transducers, following the approach detailed in the reference [11].

The numerical modeling is performed using OpenSMOKE++ [12]. Previously, the UCL mechanism was developed to predict lean and rich premixed $OME_1/O_2/Ar$ flames [10]. In this work, the kinetic model has been updated and extended by building sub-mechanisms, accounting for the formation and the consumption of oxygenated species involved in OME_2 combustion under both high and low temperatures. These oxygenated species are mainly produced by the following reaction classes: addition of O_2 to OME_2 radical ($R + O_2 \rightleftharpoons RO_2$), $R + RO_2 \rightleftharpoons RO + R'O$, peroxy radical isomerization, β scission of OME_2 radicals and so on. The mechanism has been tested on the results of the low-pressure laminar flames and the high-pressure shock tube.

Results and conclusion

In the OME_1 and OME_2 laminar flames under stoichiometric and fuel-lean conditions, good agreements were found between the simulation results with the new mechanism and experimental mole fraction profiles of reactants, products, and main intermediates (CH_2O, CH_4, HO_2, C_2H_4, etc.). Slight deviations of the simulated results from the experimental ones were observed for the mole fraction profiles of some intermediates like CH_3, C_2H_6, CH_3OCH_2, which might be due to the estimated temperature profile used in the modeling.

The prediction of the ignition delay time of OME_1 and OME_2 fuel-rich and stoichiometric combustion was found to have good performance for all temperatures studied. A deviation between experimental and simulated ignition delay time of OME_2 combustion under the fuel-lean condition was found at low temperatures, indicating the requirement for further modifications of the low-temperature reactions in the sub-mechanism of OME_2.

Thanks to the reaction pathway analysis of OME_1 and OME_2 consumption, it was concluded that H-abstraction reactions dominate OME_1 consumption, leading to the production of fuel radicals. The consumption pathway of OME_2 is consistent with that of OME_1, which would help develop the sub-mechanism of OME_3 in the future.

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