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Unravelling the Combustion and Pyrolysis Chemistry of Oxymethylene Ethers As Potential e-Fuel

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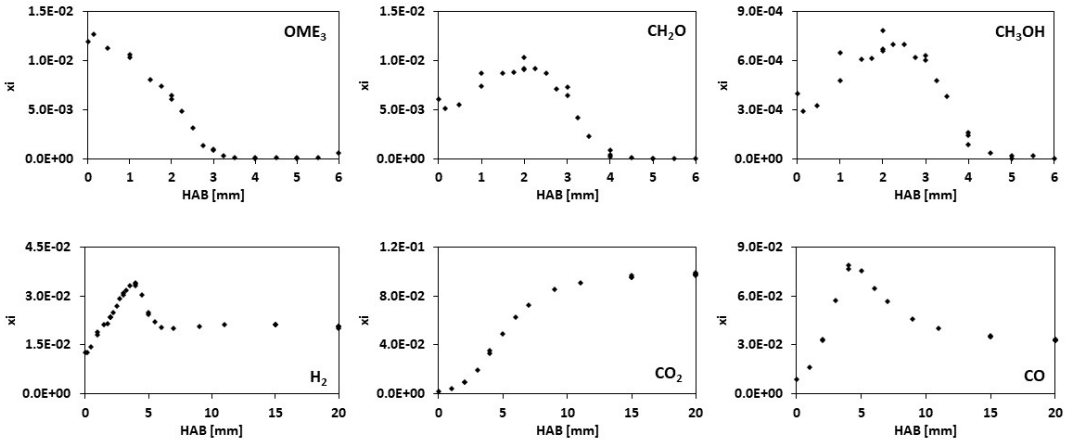
Abstract Text:
The present research focuses on the combined modeling and experimental work on combustion and pyrolysis of oxymethylene ethers (OMEs). OMEs form a promising type of synthetic fuels which can be produced via carbon capture and utilisation (CCU) in a carbon-neutral manner starting from captured CO_2 and renewable energy. Moreover, blending them with conventional diesel reduces soot emissions because of the absence of carbon-carbon bonds in OMEs. This results in less harmful emissions and contributes to a more sustainable transport sector. Both oxidation and pyrolysis microkinetic models have been constructed systematically via in-house developed automatic kinetic model generation code, called Genesys. The availability of accurate thermochemical and kinetic data is a prerequisite to construct a reliable model. Therefore, high-level ab initio calculations at the CBS-QB3 level of theory have been carried out for important reaction pathways for both low- and high-temperature oxidation of OME_3. The results of these ab initio calculations are extrapolated by regression of new group additive values and rate rules which are useful for long-chain OMEs. Both flat flame burner and rapid compression machine experiments have been performed for validation of the OME_3 combustion model. Flame experiments are performed at 0.053 bara and φ=1.0 with a fuel composition of 20 mol% OME_3 and 80 mol% CH_4. Measured concentration profiles in function of the height above burner (HAB) of some important species are depicted in Figure 1. Ignition delay times are measured via rapid compression machine experiments at 5 bara for φ=0.5 and φ=1.0. Similarly, pyrolysis experiments are performed for OME_3 on a bench-scale steam cracker setup over a broad range of temperatures (723 K – 1073 K) to validate both the primary and secondary chemistry of the pyrolysis model.



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