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A combined experimental and kinetic modeling study on pyrolysis and oxidation of polyoxymethylene dialkyl ethers

Aim

This thesis aims to investigate the radical decomposition chemistry of sustainable polyoxymethylene dialkyl ethers by means of experiments and computer-aided construction of detailed kinetic models.

Justification

Replacing fossil-based fuels with sustainably produced energy carriers has been an active research topic over the past decades as electrification is not yet feasible for heavy-duty transportation. Oxymethylene ethers (OMEs) represent a family of compounds with alternating carbon and oxygen atoms in the backbone saturated with hydrogen atoms. These molecules have high-potential properties for applications as synthetic fuel. OMEs are categorized as e-fuels since they can be produced in a carbon-neutral manner via carbon capture and utilization technology starting from captured CO_2/CO and renewable energy. However, OMEs have lower calorific heating values compared to fossil-based fuels as they are already partially oxidized. By substituting the methyl end-groups of OMEs with longer alkyl chains, the internal energy of the molecules can be increased. These polyoxymethylene dialkyl ethers (PODAE) qualify as sustainable aviation fuels (SAFs). However, before being widely applicable, it is important to understand the pyrolysis and oxidation chemistry of these compounds.

Figure 1. E-fuels as sustainable fuel for transportation applications.

Computer-aided model development for radical processes is nowadays feasible due to an increase in computational resources and fundamental knowledge. An extension of the in-house developed automatic model generation framework (Genesys) with new data for PODAEs is intended. The research can encompass both modelling and experimental aspects. A detailed kinetic model for the combustion of PODAE (in a hydrocarbon matrix) will be constructed with Genesys based on known reaction families. Accordingly, thermodynamic data and kinetic parameters are determined by on-the-fly fast estimation techniques, such as group additivity theory and artificial neural networks, as well as high-level quantum chemical calculations. Experiments can be performed on the bench scale pyrolysis unit or micro-pyrolysis unit to obtain reliable data for varying conditions to validate the final microkinetic model.

Program

- Literature survey on the applications of polyoxymethylene dialkyl ethers.
- Extension of databases with thermodynamic and kinetic parameters obtained from quantum chemical calculations and the development of fast estimation techniques.
- Automatic construction of a detailed kinetic model with Genesys for PODAEs.
- Optional: Performing experiments on the BSSC or micro-pyrolysis unit to validate and adjust the generated models.

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