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A combined experimental and modeling study on oxidation of oxymethylene ethers (OMEs) as high-potential E-fuel

Aim

This thesis aims to investigate the decomposition chemistry of oxymethylene ethers by means of computer-aided construction of microkinetic models.

Justification

Oxymethylene ethers (OMEs) are a family of molecules with alternating carbon and oxygen atoms in the backbone saturated with hydrogen atoms. These molecules have very interesting properties for applications as synthetic fuel. OMEs are categorized as e-fuels since they can be produced in a carbon-neutral manner via CCU starting from captured CO_2 and renewable energy. In addition, blending them with conventional diesel reduces soot emissions, due to the absence of carbon-carbon bonds, while still being compatible with current diesel engines. OMEs could as such contribute to the development of a more sustainable transport sector within the near-future, and a circular carbon economy in general. However, before being widely applicable, it is important to understand the pyrolysis and oxidation chemistry of these compounds and their interaction with hydrocarbons.

Figure 1. Oxymethylene ethers as sustainable fuel.

Computer-aided model development for combustion processes is nowadays feasible due to an increase in computational resources and fundamental knowledge. An extension of the in-house automatic model generation framework (Genesys) with new data for OMEs is intended. The research encompasses both modelling and experimental aspects. A microkinetic model for the combustion of OMEs 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 will be performed on the micropyrolysis setup or a bench scale reactor (BSSC) to obtain reliable data used to validate and enhance the final microkinetic model.

Program

- Literature survey on the application of synthetic fuels.
- Extension of databases with thermodynamic and kinetic parameters for larger OMEs (OME-4/5) obtained from high-level quantum chemical calculations.
- Automatic construction of a microkinetic model with Genesys for OME-hydrocarbon blends.
- Performing experiments on the micropyrolysis setup and/or BSSC to validate and adjust the generated models.

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