LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	Supervisors	Funding
Kevin De Ras	Prof. Kevin M. Van Geem, Prof. Joris W. Thybaut	FWO

A combined experimental and kinetic modeling study on oxidation of oxymethylene ethers (OMEs) as carbon-neutral fuel

Aim

This thesis aims to investigate the decomposition chemistry of oxymethylene ethers by means of experiments and computer-aided construction of kinetic 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 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. In addition, blending them with conventional diesel reduces soot emissions, due to the absence of carbon-carbon bonds, while still being compatible with the current generation of 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 interactions 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 developed 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 can be performed on the bench scale pyrolysis unit (BSSC) or micro-pyrolysis unit to obtain reliable data for varying conditions 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 quantum chemical calculations and development of artificial neural networks.
- Automatic construction of a microkinetic model with Genesys for OME-hydrocarbon blends.
- Performing experiments on the BSSC or micro-pyrolysis unit to validate and adjust the generated models.

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