LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisors**	**Collaboration**
Kevin De Ras	Prof. Kevin M. Van Geem	United States Air Force Academy

A combined experimental and kinetic modeling study on pyrolysis and oxidation of e-fuels

Aim

This thesis aims to investigate the radical decomposition chemistry of e-fuels 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 through carbon capture and utilization technology starting from captured CO_2 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 a promising fuel for the aviation sector. 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 kinetic 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 will be constructed with Genesys based on known reaction families. Accordingly, thermodynamic properties and reaction rate coefficients 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 e-fuels
- 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 bench-scale pyrolysis or micro-pyrolysis unit to validate and adjust the generated models.

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