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Coach	**Supervisor(s)**	**Funding**
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Modeling Feed Dependence of Catalytic Pyrolysis of Plastic Waste

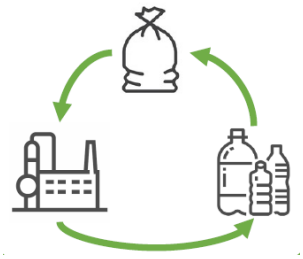
Keywords

Aim

Develop a microkinetic model which can model the ex-situ catalytic pyrolysis for both polypropylene and polyethylene to understand the effects of polymer sorting on the process.

Justification

With an annual production of 350 Mt plastics, the recycling of plastic waste will be one of the crucial challenges for the chemical industry to achieve climate neutrality [1]. *Ex-situ* catalytic pyrolysis of polyolefins is a promising technology for the conversion of waste polyolefins to high-valuable light olefins. Subsequently, these olefins can be converted into virgin polymer or other valuable base chemicals, which closes the loop for polyolefin waste.



The development of improved catalysts that enhance both the activity and selectivity towards olefins is one of the main areas of interest for the industrialization of catalytic pyrolysis. Therefore, first-principle kinetic models are developed to determine the effect of the zeolite structure, polymer feed, and process conditions. A microkinetic model should be developed to extend currently existing models to model the catalytic cracking of both polyethylene and polypropylene pyrolysis oils.

An ex-situ catalytic pyrolysis model consists of two parts, a detailed microkinetic model for small carbon numbers and a lumped model for larger species. These reaction networks comprise of paraffins, olefins, diolefins, naphthenes, and aromatics. The kinetic properties are then assigned based on Bayesian optimization, resulting in efficient microkinetic models.

Program

- Literature study on catalytic pyrolysis of polyolefin waste
- Generation of detailed reaction network and couple with lumped reaction network
- Determine optimal kinetic properties with Bayesian optimization
- Validate obtained microkinetic model for polypropylene and polyethylene pyrolysis oils

References

[1] Lange JP. Towards circular carbo-chemicals – the metamorphosis of petrochemicals. Energy & Environmental Science 2021;14(8):4358-76.