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Chemical recycling of solid plastic waste: Kinetic Modeling of Fast Pyrolysis of plastic waste

Aim

Develop a detailed understanding of the underlying reaction mechanism for the pyrolysis of solid plastic waste by means of elementary step based detailed modeling approaches and using plastic waste model compounds. Validate simulated model results through experimentation.

Justification

Polymers are so widespread all around the globe mainly because of their superior properties such as lightweight, durability, low cost, and ease of production. For more than 50 years, global production of plastics has continued to rise steadily and nowadays nearly 8% of the petroleum consumed worldwide is being used for the production of plastics. It should be critically noted that the amount of solid plastic waste (SPW) being generated goes hand in hand with the escalation of the production and utilization of plastics. The global SPW production has steadily increased over the years to reach a value of 150 million tonnes per year as reported in 2017. Conventional mechanical recycling processes are unable to process the mixed waste (and maintain its quality). In contrast, chemical recycling technologies convert the SPW into alternative fuels or useful chemicals. As they can overcome the barriers imposed by conventional mechanical recycling, they have recently gained huge academic and industrial interest.
Pyrolysis is one of the simpler, more versatile and cheaper thermochemical routes to process the SPW in the absence of a catalyst. The significant industrial from companies like DOW, TotalEnergies, Neste, and Borealis indicates the huge potential of this technology To design and optimize a suitable reactor for the pyrolysis of the SPW, it is important to understand the intrinsic kinetics and complex free-radical reaction mechanism of the pyrolysis process. Given the inhomogeneity of the SPW together with the complex product distributions, experimental and theoretical studies are generally performed starting with model compounds, such as long chain linear alkanes which can imitate linear polyethylene behavior. A single-event microkinetic (SEMK) model will help obtaining a detailed description of the radical reactions and the corresponding overall product distributions. The developed kinetic models will be coupled to artificial intelligence tools to optimize the complex set of kinetic parameters.
The model will subsequently be compared against thermogravimetric measurements, time-resolved and detailed intrinsic experimental data, obtained from the in-house micropyrolyzer setup or a dedicated pilot-scale setup. Validation data gathered from these setups will, together with the LCT's unique GC x GC-infrastructure facilitate an accurate identification and quantification of the pyrolysis products. These data will lay an ideal, though crucial, base for validating kinetic models.

Program

- Detailed literature study on pyrolysis of solid plastic waste (SPW) as well as pure and mixed polymer feedstock such as PE, PS, PU, and PP. Comprehensive understanding of the different experimental and modeling approaches for the fast pyrolysis of model plastic compounds.
- Apply and extend the currently available in-house kinetic models to accurately simulate the experimental data. Next to the degradation aspect, emphasis will be given to the reactor modeling aspect, which also includes incorporating the impact of transport phenomena, bubble formation, and volatilization.
- ANNs will be utilized for kinetic parameter tuning purposes. These tools will be extended to account for a wider range of factors (residence time distribution, *e.g.* via the *curve matching*

algorithm…) The produced models will provide insights on the key operating parameters for the scale-up of the pyrolysis process.

- Experimental study of the pyrolysis of several plastic waste and model compounds, using the LCT's dedicated experimental infrastructure (GC x GC, micropyrolyzer, pilot-scale pyrolysis setup). These data will be bundled with the developed kinetic models.