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Kinetic Modeling of Fast Pyrolysis of Solid 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 and to power plastic manufacturing processes. 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. Chemical recycling technologies, which can convert the SPW into alternative fuels or useful chemicals, are recently getting increasing attention in the scientific community. Pyrolysis is one of the simpler and cheaper thermochemical routes to process the SPW in the absence of a catalyst. To design and optimize a suitable reactor for the chemical recycling of the SPW, it is important to understand the intrinsic chemical reaction network of the fast 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. Fast pyrolysis of plastics proceeds through a free radical mechanism, which comprises of hundreds of different chemical compounds involved in thousands of distinct chemical reactions. A single-event microkinetic (SEMK) model will help obtaining a detailed description of these radical reactions and the corresponding overall product distributions. Additionally, artificial intelligence tools, and specifically artificial neural networks (ANNs), show great potential for highly complex and nonlinear problems in view of kinetic parameter tuning. Thus, the created detailed kinetic models will be coupled with ANNs to fine-tune the rate coefficients and achieve physically realistic values.
The micro-pyrolyzer setup at the LCT has been designed to study the intrinsic kinetics of plastic materials. The GC x GC and the customized RGA coupled with the micro-pyrolyzer reactor allow a detailed analysis of the pyrolysis product spectrum. Moreover, the TOF-MS with “select eV” feature enhances the molecular ion ratios, and thereby, provides accurate identification of the heavy hydrocarbons in the product stream.

Program

- Detailed literature study on pyrolysis of solid plastic waste (SPW) as well as pure polymer feedstock such as PE, PS, 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. ANNs will be utilized for kinetic parameter tuning purposes. Special emphasis will be given on the reactor modeling aspect together with the competition between volatilization and degradation. Produced models will provide insights on the operating parameters for the scale-up of the pyrolysis process.

- Experimental study of the pyrolysis of several plastic waste model compounds, using the tandem micro-pyrolyzer setup, to obtain detailed information on the product distribution and underlying reaction kinetics.