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Coach	**Supervisor(s)**	**Funding**
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Single-event modelling of the steam cracking of plastic waste pyrolysis oils

Aim

Unraveling the chemistry of components commonly found in plastic waste pyrolysis oils such as oxygenated or olefinic components.

Justification

Chemical recycling of plastic waste is expected to grow exponentially in the coming decades with plastic waste pyrolysis in particular. This process produces as the main product an oil that can be used to (partially) substitute fossil-based feedstocks to produce light olefins, with steam cracking being the most important process. The primary concern of utilizing pyrolysis oils in existing steam crackers is the substantial difference between those synthetic oils and fossil-based feedstocks for which steam crackers are originally designed. Specifically, the high concentration of heteroatom-containing contaminants (such as oxygen) and up to 60% of unsaturated hydrocarbons in typical pyrolysis oils will affect the operation and product yields of steam crackers. New reaction possibilities and the formation of unwanted products (coke precursors, methanol, NO, etc.) need to be accurately described. Furthermore, olefin producers are uncertain about the optimal conditions for cracking these plastic waste oils due to their largely different composition in terms of unsaturated components. To address these issues, the existing kinetic model CRACKSIM must be adapted for plastic waste-derived feeds, enabling fast and reliable simulation of product yields using the in-house developed simulation software COILSIM1D.

Program

1. Literature study of the thermal decomposition pathways of oxygenated and/or olefinic compounds in plastic waste pyrolysis oils under steam cracking conditions.
2. Implementing the most important reaction families in the primary reaction network generator PRIM-X.
3. Simulate the decomposition of selected components using COILSIM1D and compare them to experimental results from literature/LCT.