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Chemical recycling of polyolefin plastic waste: Kinetic modelling of the hydrothermal decomposition

Aim

This thesis aims to investigate the thermal decomposition of polyolefin plastic waste when mixed with supercritical water. This will be achieved through the development of an elementary step based model based on the well known thermal decomposition pathways of normal hydrocarbons.

Justification

Ideally the reader does not need to be convinced that plastics are everywhere; due to their low cost and flexible properties they have carved out a niche in almost every material sector. In 2020 29.5 million tons of plastic waste was collected within Europe, only 35% of which is currently being recycled. The majority of the leftover fraction is incinerated through a process affectionately named “energy recovery” which produces more CO₂ per Joule than burning coal. It is therefore evident that this is not a suitable option for a sustainable future. The 35% of plastics that is being recycled is done so through mechanical recycling, however this has almost reached its limits as mechanical recycling is unable to deal with the majority mixed plastic waste streams currently coming out of sorting facilities and often results in lower quality materials.

Chemical recycling techniques on the other hand are generally much better at handling mixed plastic waste streams as they convert them into useful chemicals or feedstocks which can be used in the production of new base chemicals. One method of chemical recycling is pyrolysis, here the polymer chains in the plastic are broken at elevated temperatures resulting a pyrolysis oil. This oil could then theoretically be fed into a cracker to produce new base chemicals. However, in practice, the oil requires extensive cleaning to remove contaminants and increase its quality before it can be fed into a cracker. This is where the supercritical water comes in: if during the pyrolysis process the plastic waste is mixed with water at high pressures it can help break down the contaminants and remove them resulting in a much cleaner oil.

Polyolefin plastic waste, i.e., PE and PP, represents the largest fraction of plastic waste due to their application in the single-use packaging industry. As such, research into their decomposition under pyrolysis conditions is of interest both academically and industrially. A single-event microkinetic model will provide insight into the radical pathways through which these polyolefins decompose. As polymers are too large molecules to be represent as a whole the decomposition mechanism will be based on the repeating unit and the chain ends. Information regarding the chain length distribution will have to be tracked through either the use of the method of moments or a lumping procedure. The developed model will be validated using experimental data gathered from literature.

Program

- Literature study in the thermal breakdown of polymers specifically PE and the possible modelling approaches that can be taken to include chain length distribution data
- Apply and expand the currently available in-house kinetic models of hydrocarbon decomposition to the decomposition of a polyolefin such as PE
- Validation of the constructed model using experimental data found in literature