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Experimental and modelling study of the hydroprocessing of caprolactam

Aim

Investigate and model the kinetics of the hydroprocessing of caprolactam via an experimental campaign in a CSTR type reactor.

Justification

The hydrocarbon industry will be facing important changes in the coming years. The inclusion of plastics and renewables in the hydrocarbon processing scenario will be managed by combining these circular feeds with fossil fractions in conventional processes such as hydroconversion. Mixing pyrolysis oil from recycled plastic with VGO as feed for hydrocracking opens an opportunity to close the loop in the plastic production process. As described in Figure 1, in this scenario the hydrocracker would maximize the yields of paraffins and iso-paraffins for the steam cracker to maximize production of ethylene and propylene that are later used to produce plastics.

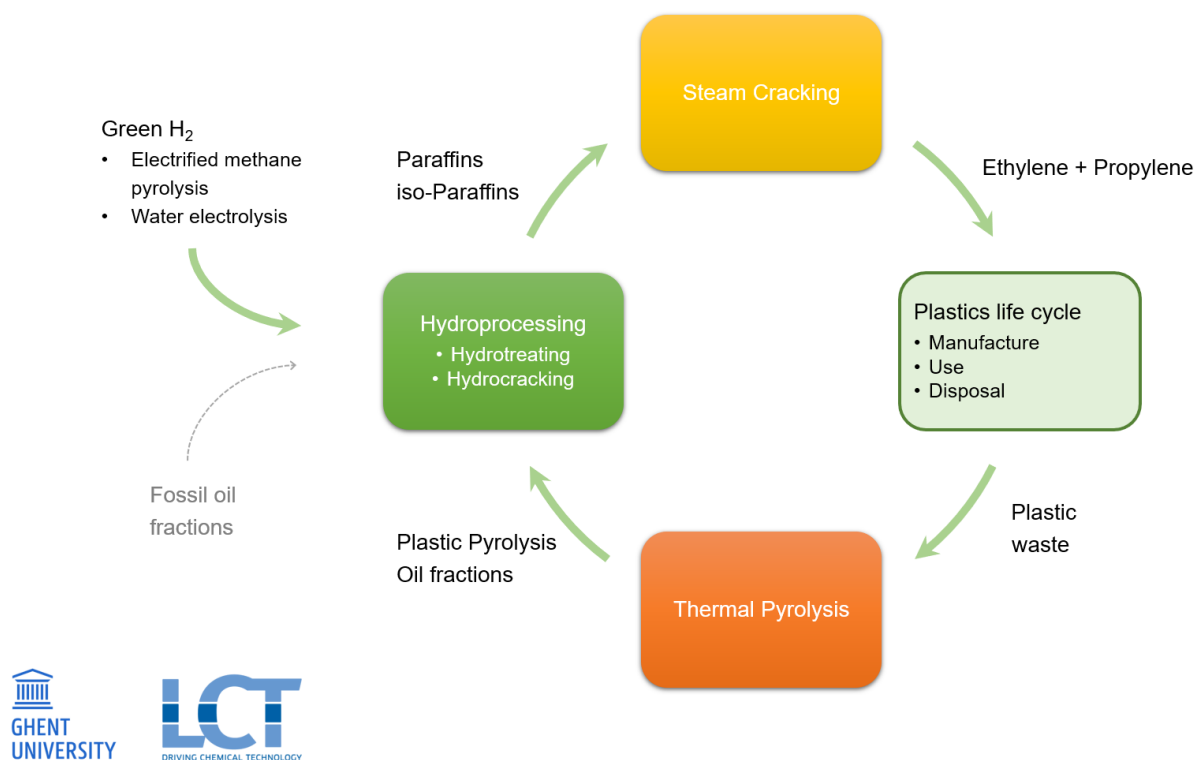


Figure 1: Circular scheme for plastics

The proportion of plastics and renewables in the combined feeds is, at least initially, limited because of potential negative impacts on the downstream processing. In particular, high concentrations of particular nitrogen containing compounds that have been identified in plastic pyrolysis oil can be detrimental for the quality of the downstream processes. Caprolactam is one of these exotic molecules contained in Plastic Pyrolysis Oil that are not present in fossil fractions.

Using an available set up at the LCT that combines a CSTR reactor with an on-line 1D GC to continuously monitor the composition of the gas stream, one of the goals of this thesis is to perform an experimental campaign that allows to treat a Synthetic Pyrolysis Oil mixture including Caprolactam. The obtained results will be used to develop a kinetic model that allow to get a more detail understanding of the mechanism of hydroprocessing of caprolactam.

Program

1. Perform a literature review about the hydroprocessing of nitrogenated compounds.
2. Plan the experiments to be execute in the Robinson Mahoney set-up.
3. Perform the experimental campaign.
4. Analyze feed and product samples using 1D chromatographic analysis.
5. Calculate the mass balance for each of the experiments.
6. Propose potential mechanisms describing the hydroprocessing of caprolactam
7. Develop and compare different kinetic models for the hydroprocessing of caprolactam.