LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
Gust Popelier	Kevin Van Geem Maarten Sabbe	FWO

Equations of State: The critical component in the modelling of supercritical water-hydrocarbon systems.

Aim

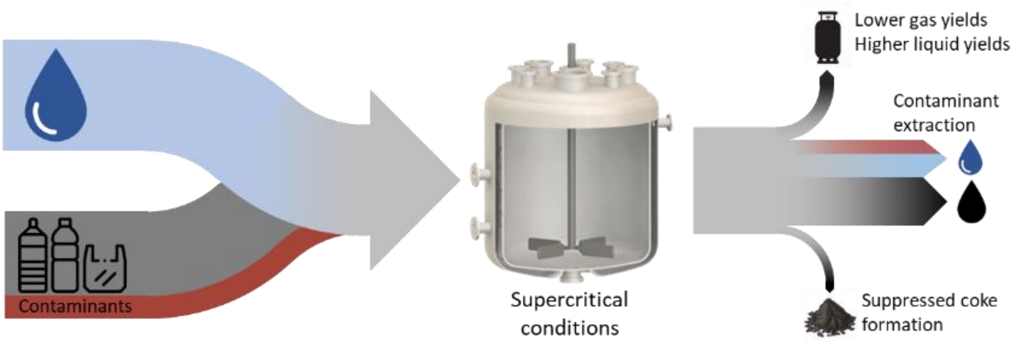
This thesis aims to investigate the interactions that occur in water-hydrocarbon systems at supercritical conditions. This will be achieved through the development of a thermodynamic model (an Equation of State) to predict the phase behavior of these systems.

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 CO_2 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 such chemical recycling technique is supercritical water pyrolysis, this is the mixing of plastic waste with water heated and pressurized to supercritical conditions resulting in the plastic decomposing to an oil. At supercritical conditions water becomes a much better solvent for hydrocarbons allowing it to partially dissolve polyolefins and their decomposition products. This results in a different environment for reaction compared to the process in the absence of water, called classical pyrolysis, and results in a higher quality oil formed at the end of the process.

This thesis will consider the water-hydrocarbon interactions that lie at the base of this process. a programming framework was developed for the practical implementation of the thermodynamic models that predict these interaction and the resulting behavior. This framework can be extended to include new or modified thermodynamic models, that better predict water-hydrocarbon interactions at supercritical conditions.



Program

- Literature study on the interactions and behavior of water-hydrocarbon systems at supercritical conditions.
- Use and expansion of a programming framework for the prediction of phase behavior and fluid properties.
- Development of a model to predict the water-hydrocarbon phase behavior at supercritical conditions.

GHENT UNIVERSITY

DRIVING CHEMICAL TECHNOLOGY