LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	Supervisor(s)	Funding
Sphurti P. Kulkarni	Prof. Kevin Van Geem	-

Integrated modelling and process simulation of the chemical recycling of polyolefins using sub- and supercritical water

Aim

The broad objective of this study is to gain a comprehensive understanding of the process involved in the degradation of polyolefins in sub- and supercritical water. Specifically, the study aims to investigate the impact of process parameters on the yields of polyolefin degradation products and develop simplified kinetic models for predicting the yields of various product groups. These kinetic models will be integrated into a global process simulation using Aspen Plus® to model the process of converting polyolefins into different hydrocarbon rich products, such as wax, oil, and gas, in sub- and supercritical water. Ultimately, this understanding will facilitate further process optimization and enable techno-economic and life cycle assessments.

Justification

Chemical recycling of polyolefins presents a promising approach to addressing plastic waste by converting polymers back into valuable products. Pyrolysis, a common method in chemical recycling, is limited in its ability to control product distribution, manage inorganic contaminants, and optimize reactor design parameters. Introducing a reaction medium such as water at high pressure and temperature (i.e., sub- and supercritical water) significantly enhances the flexibility of the process. This approach potentially can allow better control over product distribution while also facilitating the removal of inorganic contaminants in a single reaction and separation step. At sub- and supercritical conditions, water undergoes dramatic changes in its thermophysical properties, such as a significant drop in dielectric constant at supercritical conditions and the highest ionic product at subcritical conditions. These dynamic properties can be leveraged to improve process performance by dissolving non-polar products, enhancing mixing through increased diffusion, and improving overall heat transfer—key factors in reactor design and process control that contribute to a more efficient process. However, the high pressure and temperature requirements pose challenges in terms of safety, cost, and the need for precise design and optimization. Simulations can help mitigate experimental complexities, making optimization simpler and improving overall process performance.

While the development of kinetic models is an essential first step in understanding the process, there is still a lack of data over a broad range of conditions. Current literature typically explores a limited range of operating conditions (e.g., 425 to 450°C, 25 MPa), making it necessary to compare and generalize the findings across different studies to form a comprehensive understanding of the process at various temperatures and pressures. However, due to the use of different reactors and reactor volumes in these studies, direct comparisons can be misleading. A model that accounts for non-idealities, such as varying heating rates, can help normalize the data by incorporating these differences and predicting the yields reported in various studies. This model can also provide a clearer picture of the overall reaction pathways. Integrating the kinetic model with simulations will further enhance the understanding of the process and generate more data. These simulated reactors can then be incorporated into a comprehensive process simulation. The development of a conceptual process flow diagram, incorporating validated reactor models and real-world industrial processes (such as MURA Technology), will provide a more accurate foundation for process optimization, mass and energy balances, and ultimately enable realistic techno-economic and life cycle assessments.

Program

1. Conduct a literature survey and collect relevant data.
2. Develop a simplified kinetic model to predict the product distribution (using isothermal or non-isothermal models, with simulation-aided data generation if necessary) for the degradation of Polyethylene and Polypropylene in sub- and supercritical water.
3. Develop an Aspen Plus® simulation of the chemical recycling process for polyolefins using sub- and supercritical water, including the creation of conceptual process flowsheets and simulations.
4. Optional: Perform a techno-economic and life cycle assessment of the proposed process.