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Coaches	**Supervisors**	**Funding**
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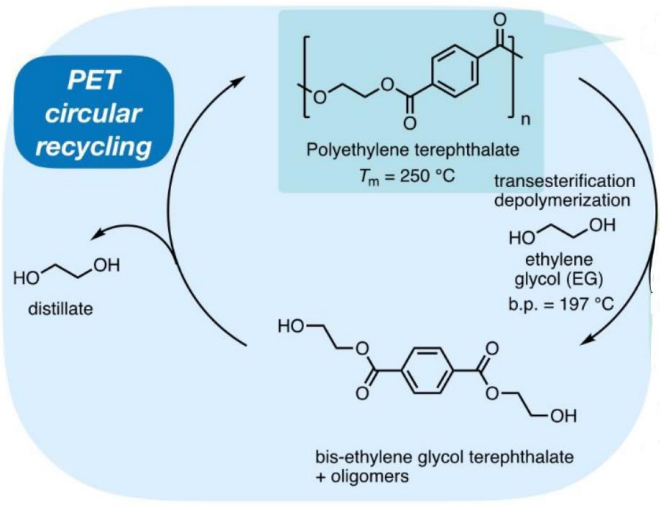
Toward achieving circularity for polycondensation products via combining experiments and simulation

Aim

Explore the potential for circularity for polycondensation products via kinetic modeling.

Justification



Over half of the annual world plastic products is comprised of polyolefins, but a large part is also represented by condensation polymers, such as polyamides, polyesters, polyurethanes and polycarbonates. The societal challenge is to close the carbon cycle by converting this plastic waste polymer mass into either monomers or higher value oligomers, which can then be reused in upcycling or recycling processes. Promising routes to increase the reusability of the carbon skeletons of major condensation polymers are novel catalysts at low temperatures and novel reactions at high temperatures. An engineering challenge lies in understanding the chemistry (side reactions; thermodynamic equilibrium), transport phenomena (multiphase medium), and the role of non-idealities such as the presence of various additives (dyes, stabilizers, volatiles, etc.) in the plastic waste.

Program

1. Literature study
2. Carrying out dedicated (small timescale) experiments using GPC, NMR, GC, FTIR characterization
3. Performing kinetic studies to determine important rate coefficients
4. Development of a Predici computer model for the efficient model-assisted repolymerisation
5. Validating the model against the experimental data, to explore the feasibility for re-/upcycling
6. Constructing a proof-of-concept kinetic Monte Carlo model to visualize (de)polymerization