LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 914, 9052 Gent, Belgium

Supervisor	**Period**	**Funding**
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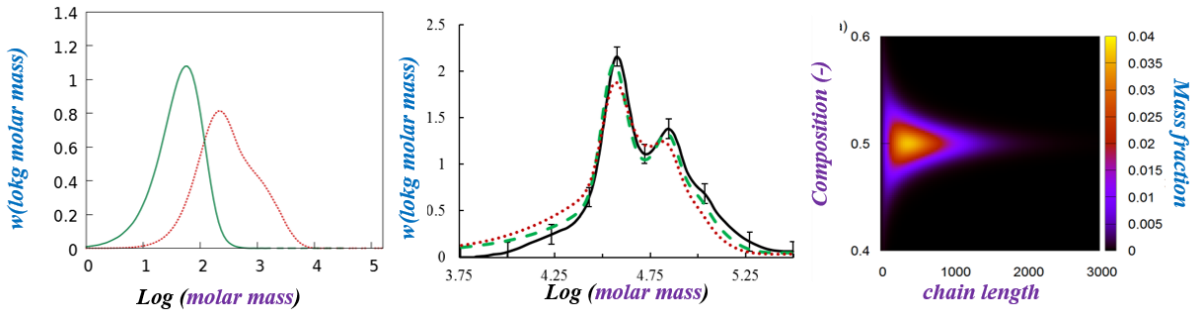
Controlling polymerization kinetics up to high chain lengths

Aim

A generic, fast and reliable kinetic modeling platform is developed, allowing the design of chain and step growth polymerization processes over the complete range of industrially relevant chain lengths. The model will be applied for both polymer reaction engineering and polymer processing applications.

Justification

In everyday life one of the most important materials are polymers, which are used both for commodity (*e.g.* household goods and packaging industry) and high-tech applications (*e.g.* drug delivery and photovoltaics). One of the key ways to tune polymer properties is controlling the chain length distribution (CLD) or molar mass distribution (MMD) during the synthesis. As shown the figure below, the MMD can be stretched out from very low molar masses to very high ones. In general, chain lengths from 1 to 10^4 or even 10^5 can result. In many applications, a broad but well-defined CLD is needed with low chain lengths leading to plasticity, allowing further shaping during polymer processing, and higher chain lengths guaranteeing strength for the processed product. On the other hand, a narrow CLD with almost identically tailored macrospecies can be required for high-tech applications. It is clear that significant improvement is still need on both the experimental and modeling level, in particular for more complex polymerization processes.



Program

1. Evaluation of current modeling tools to characterize CLDs/MMDs
2. Development of universal modeling tool in view of 1.
3. Application of modeling tool developed in 2 for a broad range of application ranges.

Several publications are envisaged in leading journals in the chemical engineering and polymer science research field.