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Molecular design for industrial copolymerization: bridging computational chemistry and pulsed laser polymerization

Aim

Improving kinetic parameters for radical copolymerization processes to enable a joint control of polymerization rate and compositional drift.

Justification

Radical copolymerization is an important process in the chemical industry as polymer materials can only be fully exploited if one can combine different molecular properties in the backbone for which the use of comonomers is an ideal strategy. A challenge with comonomer units remains the understanding of their incorporation according to a given pattern, e.g. more random, alternating or block-like. This is challenging as penultimate effects exists, implying that the addition of a monomer A to a (macro)radical ending on an A radical unit can also depend if before that unit an A or B unit is present.

Industrially, we still need to shift from so-called terminal models (only the last unit) to so-called penultimate models (not only the last unit), knowing that a penultimate effect largely effects the polymerization rate and control over the composition and thus the economic-performance balance. However, more kinetic parameters are then needed and those need to be sufficiently reliable before the industry will abandon the default attitude of terminal models.

The current Master thesis uses the leading pulsed laser polymerization (PLP) unit as available at LCT (prof. D'hooge) to provide dedicated experimental data on copolymerization propagation parameters to compared terminal and penultimate models. The interpretation is supported by computational chemistry tool application, a key expertise of CMM (prof. Van Speybroeck) further supported by complementary knowledge on PLP and copolymerization kinetics at LCT (prof. D'hooge, prof. Sabbe and Dr. Marien).

Program

1. Literature study on the relevance of PLP for copolymerization kinetics of industrially relevant comonomer pairs. Selection of interesting comonomer pairs for benchmark and industrial application.

2. PLP and polymerization study (LCT) to quantify copolymerization kinetics, specifically homo- and crosspropagation Arrhenius parameters.

3. Interpretation of PLP data supported by computational chemistry (CMM) to pinpoint the ideal conditions to design both the rate and compositional control.