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Pulsed laser (co)polymerization to enhance industrial polymer synthesis

Aim

The determination of essential intrinsic rate coefficients for industrial radical (co)polymerization using pulsed laser polymerization experiments and simulations.

Justification

To optimize industrially applied radical polymerization processes and to develop new polymeric materials kinetic modeling is indispensable. The success of kinetic modeling for these purposes depends largely on the accuracy of the intrinsic rate coefficients used. Since the joint estimation of these coefficients by multi-response regression to polymerization data is very demanding, an independent step-by-step determination is beneficial. Pulsed laser polymerization (PLP) is a very interesting well-accepted technique in the industrial community, allowing to study individual reactions (*e.g.* Marien *et al.*, *Advances in Chemical Engineering* 2020, 56, 59). In PLP, photoinitiator radicals are generated at laser pulses with a frequency *v* (Figure 1; left). Depending on the PLP conditions and the monomer type, the molar mass distribution (Figure 1; right) can possess specific characteristics (*e.g.* repetitive inflection points), allowing the determination of intrinsic rate coefficients (*e.g.* Marien *et al*. *Macromolecules* 2017, 50, 1371 and Vir *et al*., *Polymer Chemistry* 2019, 10, 4116).

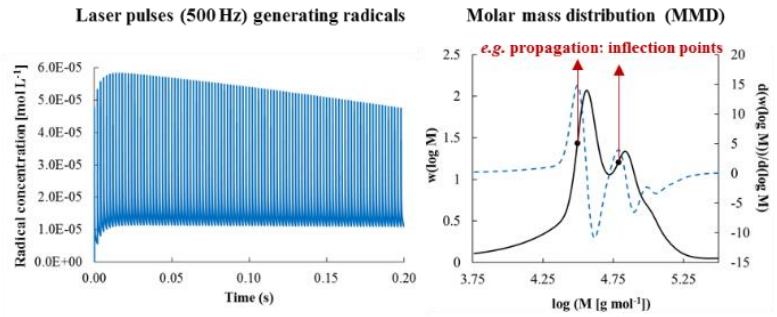

Figure 1. Radical concentration profile (left) and molar mass distribution (full black line; right) allowing the determination of the propagation rate coefficient via the inflection points, which correspond to maxima of the derivative (dotted blue line).

In this thesis, PLP is used for the determination of backbiting, *β*-scission and (cross)propagation rate coefficients that are essential to design industrial (co)polymerizations. Kinetic Monte Carlo (*k*MC) modeling is applied for the identification of optimal PLP conditions. Experimental data is obtained using the LCT PLP setup. (co)Monomers are selected in collaboration with industry.

Program

i. Performing a literature study on the available methods for the determination of individual rate coefficients in radical (co)polymerization.
ii. An available computer code for the kinetic modeling of PLP is used to relate specific reactions to characteristics of the PLP molar mass distribution as a function of the PLP conditions.
iii. Experimental determination of intrinsic rate coefficients for industrial radical (co)polymerization processes using the LCT PLP setup and insights obtained in (ii).

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