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Experimental study of the rate coefficients of the polymerization of modified acrylics and model development

Aim

Defining the rate coefficients of the free radical propagation reaction and side reactions in the polymerization of promising acrylic monomers (isobornyl acrylate and vanillin acrylate) and reactivity ratios in their co-polymerizations to create a model that is able to predict the molecular properties of the polymer produced by the respective polymerization reactions.

Justification

Free radical polymerization is one of the most industrially applied methods to produce polymers. In the first place, this enables the production of commodity plastics, such as polyethylene and polypropylene, used for packaging and household products. However, also specialty polymers can be synthesized via FRP when working with specific monomers such as modified acrylics. Isobornyl- and vanillin acrylate are examples of this. These monomers are interesting because of their biobased nature. Moreover, they possess antibacterial properties which might make them useful for high end medical applications.

The challenge in the development of these isobornyl- and vanillin acrylate based polymers lays in the predictability of the reaction outcome, namely the molecular properties of the (co-)polymer, since not only propagation, but also side reactions such as backbiting and beta-scission can occur. Moreover, when producing a co-polymer, knowledge of the reactivity ratios of each monomer will be crucial to predict the composition of the final product.

At LCT a Pulsed Laser Polymerization set-up is available which enables the study of the propagation and side reactions of the free radical polymerization in controlled circumstances at low conversions. A Gel Permeation Chromatograph is available to study the chain length distributions of the produced samples. This will enable the development of a complete set of Arrhenius parameters for the polymerization of these acrylics, which can be used later on in a model to predict the polymerization outcome depending on the reaction conditions.

Program

1. Literature review on modified acrylics
2. Performance of PLP and GPC experiments under specific conditions to define propagation and side reaction kinetics at different temperatures and solvent fractions
3. Preliminary model development for modified acrylics