Copiride : anionic polymerisation of 1,3-butadiene with low PDI in a continuous flow setup

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Abstract title	COPIRIDE: ANIONIC POLIMERISATION OF 1,3-BUTADIENE WITH LOW PDI IN A CONTINUOUS FLOW SETUP
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CoPI*RIDE* is a flagship “Future Factory” project in the 7th Framework Program of the EU (www.copiride.eu). The entire goal of the project is processes intensification (PI) by increasing space-time yield (STY) while keeping product specification. Higher STY allows a compact design of the reactor to integrate it into a module that fits in a compact container infrastructure. The so-called Evotrainer includes the whole process as an enclosed system. Because of its standard size it is easy to ship it to the markets or to where the educts are cheap. Improved PI is demonstrated on the example of anionic polymerisation.

Anionic Polymerisation of 1,3-Butadiene – “Batch to Conti”

Living Anionic Polymerisation (LAP) provides tailor-made polymers with a defined microstructure, molar mass and low polydispersity (PDI). Usually this type of polymerisation is performed in semi-batch reactors, but is often limited by comparatively low heat, which causes reactor runaway in extreme cases. In contrast, reactions in micro-reactors can be performed at high concentrations and high temperatures due to their excellent heat transfer rates and pressure stability. But so far the PDIs of the polymers produced in continuous flow systems do not achieve the low PDIs of batch-made polymers.

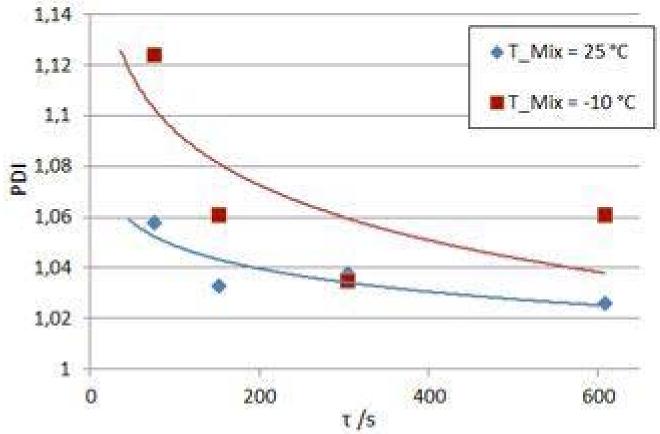
In this work, the influence of reactor geometry and mixing and reaction temperature on the product PDI is investigated for an anionic polymerisation with liquid 1,3-butadiene as monomer. Experimental results for styrene as monomer LAP-made polymers with PDIs below 1.1 can be obtained in micro structured reactors. Simulations of B. Cortese et al.suggest that segregated streamlines in laminar flow regime should be responsible for the low PDIsif the reactor is long enough to ensure full conversion over the outlet cross section. Theoretically PDIs of 1.03 can be reached.

In a novel setup design that provides a pulsation-free feed of initiator and monomer the influence of reactor geometry, residence time and feed and mixing temperature on product properties were investigated.

Polybutadienes with a PDI well below 1.1 and a molecular weight up to 30,000 g mol^{-1} could be obtained in a mili-/micro structured reactor with reasonable degree of conversion. The results offer valuable clues for an optimal reactor diameter and length of the capillary and give an indication for the segregation inside the capillary.

A successful transfer of a semibatch process to a scalable (numbering-up) continuous flow design is presented in due consideration of keeping the product quality (PDI). The dependency of product PDI on mixing temperature, residence time and capillary diameter are presented, which were used to validate the segregation model for this process.

Images



PDIs of polybutadienes in dependency of residence time.

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