

# CFD based optimization of anionic polymerization in micro flow

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# 62nd Canadian Chemical Engineering Conference

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**CFD Based Optimization of Anionic Polymerization in Microflow B. Cortese** <b.cortese@tue.nl>, M.H.J. de **Croon** < M.H.J.M.de.croon@tue.nl> and **V. Hessel** < v.hessel@tue.nl>, Eindhoven University of Technology, The Netherlands.

Anionic polymerization is an industrially relevant technique for the synthesis of polymers with highly controlled properties. Besides, especially in the last decade, due to the advances in process intensification and in miniaturization a modular chemical plant is becoming feasible. The aim of our research is the development of a deeper understanding of the interplays between the properties governing the fluid-dynamic and the reactive behavior of a micro-flow-anionic-polymerization in order to obtain the needed knowledge for the optimization of a dedicated micro-fluidic system.

To do so a model that consider the dependence of the basic physicochemical properties from the polymer weight and concentration was developed. This yielded a comprehensive insight of the flow pattern inside the reactor and of its effects has on the final product quality. A key result here is the presence of highly segregated streamlines, even at the very low characteristic length of microfluidic devices (which are usually regarded as almost perfectly mixed). The simulation results were successively validated against experiments.

The outcome was then used as a starting point for the design of a reactor that can match industrial needs while fitting into a modular infrastructure (e.g. the so-called EvoTrainer).

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