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Optimization of Microchannel Geometry for Synthesis of Polystyrene in a Microreactor using COMSOL

Abstract

Among all available methods for polymer synthesis, anionic polymerization holds many advantages that makes synthesis of polymers of well-defined end structures easier. Unlike other methods of polymer synthesis, this method lacks a formal termination step, which provides an opportunity to functionalize end-groups. However, when using conventional batch reactors, anionic polymerization typically must be carried out under strictly dehydrated and cryogenic conditions, making this method untenable for many industrial-scale applications [1]. However, using flow microreactors, the aforementioned conditions are no longer required. In addition, use of flow microreactors offers several other advantages including faster mixing, better temperature control, and more control over the molecular weight distribution of the polymer [2]. In this study, COMSOL Multiphysics software is used to model the anionic polymerization of styrene in a microreactor. The effects of various microchannel geometries on diffusion and mixing of reagents are tested to determine the optimal microchannel geometry for the reaction.

References

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