

Molecular Weight Distribution prediction model for autoclave reactor by incorporating Kinetic Monte Carlo method with Computational Fluid Dynamics model

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In previous research, several approaches are introduced to predict MWD for different kinds of reactors such as batch reactor, CSTR and PFR. Those proposed models consume reactor to be homogeneous, but none of the model takes into account imperfect mixing in reactor. However, the mixing is essential to enhance the rate of mass transfer and polymer coagulation, so that it makes significant difference in MWD compared to homogeneous cases.

In this research, we develop new approach to predict MWD for inhomogeneous reactor. We adopt Kinetic Monte Carlo method and incorporate it with flow data which directly provides information about micro-mixing. Flow data is obtained from CFD model which is divided into 214 compartments by extracting flowrate between each compartment. The model is validated with real MWD data of Ethylene-Vinyl acetate copolymer autoclave reactor. Research represents the effect of mixing on MWD, so it can provide reasonable idea for designing reactor which desired property of polymer can be obtained from.