

A Study of Molecular Weight Distribution of Polyethylene by kinetic Monte Carlo Simulation

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It is noted that commercial polyethylene polymers produced by autoclave reactor have a special property, a 'molecular weight distribution (MWD) shoulder.' There are just few precedent researches that explain how it was made. I assumed two major causes, mechanical issue and kinetic issue, of it and confirmed it through kinetic Monte Carlo (kMC) Simulation. I considered the mechanical issue as imperfect mixing effects and kinetic issue as effects of the autoclave reactor's high temperature and pressure and made it as a equations in my kMC Simulation.

The simulation will be conducted with case analysis of several conditions, so the result of it will let us know the effects of imperfect mixing effects and autoclave reactor conditions in a formation of MWD shoulder.