

MODELING POSSIBLE LONG CHAIN BRANCHING REACTIONS FOR POLYETHYLENE IN A SEMI-BATCH REACTOR

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Key Words: long chain branching, constrained geometry catalyst, C-H activation, ethylene polymerization modeling, terminal branching

Long chain branches (LCBs) in polyethylenes made with metallocene catalysts are conventionally accepted to be formed via random terminal branching reactions. However, other reactions such as C-H activation and intramolecular incorporation have been suggested in the literature as alternative pathways to LCB. In this simulation work, we contrasted two possible mechanisms for LCB formation in a semi-batch reactor: terminal branching and C-H activation to find out how different polymerization conditions and LCB mechanisms affected the polymer microstructure. The C-H activation reaction was broken down into 3 steps: bond activation of a dead chains, bond activation of macromonomers (dead chains with terminal vinyl groups), and bond activation of a living chain (intramolecular pathway). As it is quite difficult to determine which C-H bond activation reactions (if any) are relevant to LCB formation in these systems, we compared all possible scenarios to distinguish which are more likely to make polyethylenes with the microstructures observed experimentally in terms of molecular weight distribution, long chain branching density, and branching as a function of chain lengths for the different polymer species in the reactor.