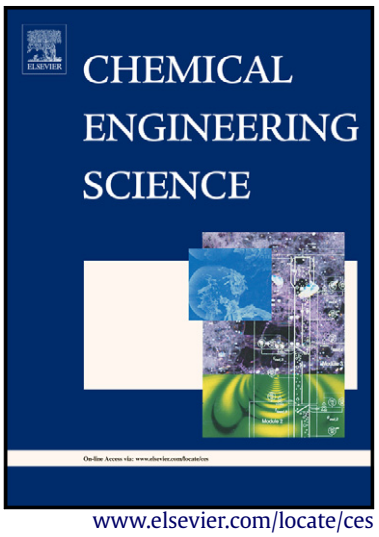

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Molecular weight/branching distribution modeling of low-density-polyethylene accounting for topological scission and combination termination in continuous stirred tank reactor

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Abstract

We present a comprehensive model to predict the molecular weight distribution *(MWD)*[1], and branching distribution of low-density polyethylene *(ldPE)*[2], for free radical polymerization system in a continuous stirred tank reactor *(CSTR)*[3]. The model accounts for branching, by branching moment or *pseudo distributions*. The common free radical polymerization reactions including chain scission have been considered in the model. *Non-linear* or the so-called *topological* scission has been modeled using approximate *fragment length distributions* derived from scission, applied to branching topologies. To model the distributions, the Galerkin-FEM method based on the same principles as PREDICI® has been applied and implemented in MATLAB©. The fundamental numerical problem arising from topological scission has been solved. Thus, the model provides more accurate results, allowing a precise comparison to earlier results and to Monte Carlo simulations.

Keywords:

Free radical polymerization, Reaction engineering, Molecular architecture design, Product design, Galerkin FEM, Hypergeometric distribution

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1 Molecular Weight Distribution

2 low density PolyEthylene

3 Continuous Stirred Tank Reactor