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Predicting Polyethylene Processing Properties Based on Reaction Conditions via a Coupled Kinetic, Stochastic and Rheological Modelling Approach

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Abstract : Being able to predict polymer properties and processing behavior based on the applied operating reaction conditions in one of the key challenges in modern polymer reaction engineering. Especially, for cost-intensive processes such as the high-pressure polymerization of low-density polyethylene (LDPE) with high safety-requirements, the need for simulation-based process optimization and product design is high. A multi-scale modelling approach was set-up and validated via a series of high-pressure mini-plant autoclave reactor experiments. The approach starts with the numerical modelling of the complex reaction network of the LDPE polymerization taking into consideration the actual reaction conditions. While this gives average product properties, the complex polymeric microstructure including random short- and long-chain branching is calculated via a hybrid Monte Carlo-approach. Finally, the processing behavior of LDPE -its melt flow behavior- is determined in dependence of the previously determined polymeric microstructure using the branch on branch algorithm for randomly branched polymer systems. All three steps of the multi-scale modelling approach can be independently validated against analytical data. A triple-detector GPC containing an IR, viscosimetry and multi-angle light scattering detector is applied. It serves to determine molecular weight distributions as well as chain-length dependent short- and long-chain branching frequencies. 13C-NMR measurements give average branching frequencies, and rheological measurements in shear and extension serve to characterize the polymeric flow behavior. The accordance of experimental and modelled results was found to be extraordinary, especially taking into consideration that the applied multi-scale modelling approach does not contain parameter fitting of the data. This validates the suggested approach and proves its universality at the same time. In the next step, the modelling approach can be applied to other reactor types, such as tubular reactors or industrial scale. Moreover, sensitivity analysis for systematically varying process conditions is easily feasible. The developed multi-scale modelling approach finally gives the opportunity to predict and design LDPE processing behavior simply based on process conditions such as feed streams and inlet temperatures and pressures.

Keywords : low-density polyethylene, multi-scale modelling, polymer properties, reaction engineering, rheology
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