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Reaction-embedded CFD Simulation of Autoclave High-pressure Polyethylene and EVA

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Extended Abstract

Autoclave reactor is widely used to produce polymers that have special structures and performances. Coupled process of polymerization (or co-polymerization) and hydrodynamics in the reactor necessitates fundamental understanding to improve the product quality. Since these autoclave reactors usually operate at very high pressure, typically about 150-300 MPa, experimental study on such reactive flow systems is quite limited. While computational fluid dynamics (CFD) simulation provides a promising way to reveal the relationship between reactor geometry, operating conditions and key factors of the product, such as molecular weights distribution (MWD) and monomer conversion. Fields distribution of flow and temperature can be also obtained through hot-state simulation, which can be used to optimize the reactor design and operation.

This work aims at developing a reaction-embedded CFD framework for autoclave low-density polyethylene (LDPE) and ethylene vinyl acetate copolymer (EVA). First, referring to previous work [1], an industrial autoclave was studied without heat transfer and reaction. Then, the LDPE case studied by [2-3] was simulated for validation, and the simulated temperature, monomer conversion and MWD agreed well with the literature results. The method was then applied to the industrial LDPE autoclave and reasonable results were obtained according to plant data, with a temperature range of 308-535 K and the monomer conversion of 13.7%. Furthermore, co-polymerization reaction for EVA [4-5] was integrated to the CFD framework. However, simulation of individual autoclave reactor failed to capture the in-situ feature, because actually two autoclave series were used in the plant. So, we connected the autoclave series in simulation, that is, the average concentrations of each component at the outlet of autoclave A were assigned to the inlet of autoclave B. Since this change is closer to the physical reality, it obtained consistent MWD results with the plant data, where error is only about 4.39%. Then other fields prediction can be regarded credible, which enables further optimization of the reactor geometry and operating conditions.

In addition, predicting MWD and branching distribution (BD) is of crucial importance for polymer process design and improvement. Various methods have been used to cope with MWD prediction, including moment methods, Monte Carlo simulation, Galerkin methods and so on [6]. However, it is complex to deal with polymer branching structures. Different from available algorithms, we propose a novel way to calculate both MWD and BD under a steady-state framework. The new method sequentially considers radical polymerization reactions and prioritizes β-scission reaction over the chain transfer to polymer (CTP) reaction in dead polymers. Moreover, in order to avoid other empirical treatments in the calculation, an assumption between the reaction frequency and the proportion of molecules undergoing that reaction is proposed. The calculation demonstrates that MWD and BD as well as their dependence on β-scission and CTP reactions can be well predicted.

In this work, the open-source CFD software platform OpenFOAM is used, which is different from previous simulating work. Although the CFD framework and the steady-state MWD method are still in a preliminary stage, we believe that the framework developed here can be applied to more polymer producing scenarios in the future.

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