TNChE Asia 2023 Conference

COP Name XXXXXXXXXXXX

Presenter Bio data & Abstract

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Presentation Topic : **Advances in Multiscale Modeling of a Multizone Circulating Reactor: Scaling Up with First Principle Models**

Presentation Abstract:

A multiscale steady state modelling framework of a multizone circulating reactor (MZCR) is developed for propylene homo- and copolymerization with supported Ziegler−Natta (ZN) catalysts. The proposed MZCR model includes comprehensive kinetic modelling, thermodynamic modelling (accounting for non-ideal binary mixtures and co- and anti-solvent effects), and a steady-state reactor model (overall material and momentum balances, particle size distribution (PSD), and the particle residence time distribution (RTD)). In addition, the reconstruction of the cumulative molecular weight distribution (MWD) and chemical composition distribution (CCD) produced in the MZCR using a single-site ZN catalyst is provided. The new model of the MZCR was first validated with the available literature (pilot scale, — using simplified kinetics and Henry's law) to ensure mass and momentum balances. We then showed the impact of the model improvements (i.e., complete kinetics, and either a detailed Sanchez-Lacombe equation of state or simple ternary correlations). Simulation results showed a good agreement with the reference data. It was found that adding the complete kinetic model and thermodynamic model decreased the production rates due to the inclusion of deactivation reactions and dormant site effects and co- and anti-solvent effects. Finally, we used the model to simulate the commercial-scale MZCR reactor, based on available MZCR patents. When model predictions are compared to available patent data, the proposed model is shown to be capable of describing the MZCR performance in a large-scale operation, as well as predicting the monomodal (in case of PP blend) and bimodal (RCP and HPP) shapes of the MWDs.