MODELLING OF A MULTIZONE CIRCULATING REACTOR FOR PROPYLENE POLYMERIZATION: IMPACT OF THERMODYNAMIC MODEL

Kusuma Kulajanpeng, Université Claude Bernard Lyon 1, CPE Lyon, CP2M, Villeurbanne, France;
SCG Chemicals Public Company Limited, Bangkok, Thailand
kusumaku@scg.com
Nida Sheibat – Othman, Université Claude Bernard Lyon 1, LAGEPP, Villeurbanne, France
Wiwut Tanthapanichakoon, SCG Chemicals Public Company Limited, Bangkok, Thailand
Timothy F.L. McKenna, Université Claude Bernard Lyon 1, CP2M, Villeurbanne, France

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Thermodynamics of sorption equilibrium in gas-phase catalytic polymerization of α-olefin play a key role in the polymerization rate and polymer properties, especially when co-solubility and anti-solubility are significant.[1] Individual and total solubilities of multiple penetrants (i.e., propylene, propane, and their mixtures) in amorphous isotactic polypropylene (iPP) are measured at industrial relevant conditions (i.e., temperature of 75 °C and 85 °C, and pressure range of 0 – 20 bar) using a pressure decay method. The obtained solubility results are correlated with the Sanchez-Lacombe equation of state (SL EoS model)[2] to determine temperature-dependent binary interaction parameters (k_{ij}). The measured solubility results showed that the total and individual solubilities of gases in amorphous iPP increased with an increase in the pressure and a decrease in the temperature. It was found that the propylene solubility with the presence of propane (ternary solubility) is lower than the pure propylene solubility (binary solubility) due to the anti-solvent effect of propane on propylene. Vice versa, propylene also acts as an anti-solvent to propane, resulting in lowering propane solubility as well. Santos et al.[3] developed an isothermal and dynamic mathematic multizone circulating reactor (MZCR) model (fraction based model) for propylene homopolymerization in pilot scale. Nonetheless, Henry's law (neglecting non-ideal behaviors and the co- and antisolvent effects) was used. This work focuses on the development of a steady state model of the MZCR for propylene homopolymerization with supported Ziegler−Natta catalysts. The developed (concentration-based) model has been validated with the simulation results of Santos's pilot-scale model to ensure mass and momentum balances. Then, we improved the thermodynamic model by incorporating the SL EoS ternary model together with the obtained k_{ij} to take into account the antisolvent effects of propane on propylene and vice versa. Model predictions of monomer concentration profile in the downer (Figure 1a), and particle size distribution (PSD) at the downer outlet (Figure 1b) in the downer show good agreement with the reference data.[3] The impacts of the SL EoS ternary model is compared with the Henry's model. It can be seen that adding the SL EoS ternary model provides less propylene consumption (Figure 1a) due to the anti-solvent effect of propane as a result of decreasing in production rate in the riser (Figure 1c), the PSD (Figure 1b) moves to the left indicating smaller particles are produced due to the lower production rate.

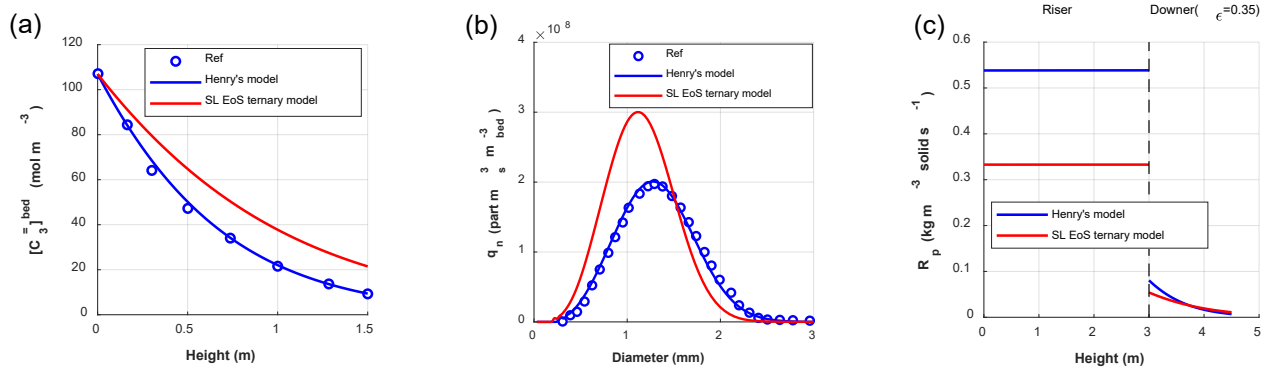

Figure 1 Comparison of the impacts of the SL EoS ternary model with the Henry's model; (a) Monomer concentration in the downer, (b) PSD at the downer outlet, and (c) Polymerization rate in the riser and the downer

References

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