J Math Chem (2012) 50:1060–1078
DOI 10.1007/s10910-011-9949-6

ORIGINAL PAPER

Coupled single-particle growth and kinetics modeling for styrene polymerization over silica-supported metallocene catalyst

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Received: 31 August 2011 / Accepted: 29 November 2011 / Published online: 6 December 2011

Abstract A comprehensive mathematical model for styrene stereoregular polymerization was carried out. This model was generated by coupling the single particle growth model (SPGM) with kinetics model, to predict the effect of intraparticle mass transfer resistance and initial catalyst size on the polymerization kinetics. SPGM was derived based on a modified multigrain model (MMGM) to calculate the spatial-time evolution of styrene concentration under intraparticle mass transfer limitations. Then, the SPGM was solved simultaneously with kinetics model to estimate the polymerization rate and molecular weight distribution (MWD) under the above mentioned limitations. The results show that a significant radial distribution of styrene concentration across polymer growing. Moreover, the diffusion resistance was most intense at the early step of the polymerization and the effects of the polymerization rate are more strongly. Additionally, it is appear that increasing the initial catalyst size leads to a decrease in the rate of polymerization. For MWD, the model simulation show that the diffusion resistance led to have an increase in the molecular weight within a period of time similar to the one needed in the catalyst decay. The validation of the model with experimental data given a agreement results and shows that the model is able to predict monomer profile, polymerization rate, and MWD of syndiotactic polystyrene.

Keywords Modeling · Particle growth · Polystyrene · Metallocene catalyst · Stereoregular polymerization

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