Iran Polym J (2012) 21:423–433
DOI 10.1007/s13726-012-0045-y

ORIGINAL PAPER

Combined single particle growth and population balance modeling in stereoregular polymerization of styrene

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Received: 8 October 2011 / Accepted: 21 April 2012 / Published online: 11 May 2012

Abstract Modeling and experimental analysis for syndiospecific polymerization of styrene over silica-supported metallocene catalyst was carried out. A detail model was developed by coupling the single particle growth model (PGM) with particle population balance equation. The model was employed to predict the effects of intraparticle mass transfer limitations and the initial catalyst particle size on the rate of polymerization and the particle size distribution (PSD) of syndiotactic polystyrene (sPS). The single PGM, based on a modified polymeric multigrain model, was first utilized to calculate the single particle growth rate and polymerization rate under intraparticle mass transfer limitations and different initial catalyst particle sizes. Then, the model was solved simultaneously with particle population balance equation to estimate the PSD of sPS under the same limitations. The single PGM results showed a significant radial distribution of styrene concentration across polymer growth. It was further noticed that the diffusion resistance was most intense at the beginning of the polymerization reaction and the effects of polymerization rate were stronger. Moreover, it appeared that increasing the initial catalyst particle size led to lower rate of polymerization. The PSD simulation results revealed that the mass transfer limitation, as well as the initial catalyst particle size made a strong impact on the PSD of sPS. In addition, the simulation results obtained from this model showed good agreement results with experimental data of sPS.

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Keywords Particle size distribution · Single particle growth · Mass transfer · Polystyrene · Stereoregular polymerization

List of symbols

$D_{e,i}$	Effective macroparticle diffusivity, at the *i*th grid point (cm^2 min^{-1})
D_1	Monomer diffusivity in pure polymer (cm^2 min^{-1})
k_p	Propagation rate constant (L mol^{-1} h^{-1})
k_d	Catalyst deactivation rate constant (h^{-1})
k_{tM}	Chain transfer to monomer rate constant (L mol^{-1} h^{-1})
$k_{t\beta}$	β-Hydrogen elimination rate constant (h^{-1})
k_1	Liquid film mass transfer coefficient (m^2 s^{-1})
M_i	Monomer concentration in the macroparticle, at the *i*th grid point (mol L^{-1})
M_b	Bulk monomer concentration (mol L^{-1})
M_0	Initial monomer concentration (mol L^{-1})
N	Number of shell
r	Radial position at the macroparticle level (m)
$R_{c,i}$	Radius of catalyst subparticles (m)
R_{N+2}	Macroparticle radius (m)
R_0	Initial catalyst particle radius (m)
$R_{h,i}$	Radius of *i*th hypothetical shells
$R_{p,i}$	Rate of reaction per unit volume at the *i*th grid point [mol(m^3 s)$^{-1}$]

Introduction

Syndiotactic polystyrene (sPS) is a latest polymeric material of industrial importance. The high crystallization rate and the high melting point (270 °C), make this polymer a