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Multiscale modeling of syndiospecific styrene polymerization

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Abstract A detailed mathematical model for syndiospecific styrene polymerization based on combining features of the multigrain model (MGM) and the polymeric multigrain model (PMGM). This model has been established to predict the radial monomer concentration within the growing macro particles and the rate of polymerization. The latter, the parameters, have an effect on the molecular weight distribution (MWD). In this model, the effect of intraparticle diffusion resistance and the radius of catalyst particles on the rate of polymerization and MWD were studied. The model simulation showed the presence of a large distribution of monomer concentration across the radius of particles. It was further noticed that the diffusion resistance was most intense at the beginning of the polymerization process. For MWD, the model simulation showed that the existence of 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. Moreover, the validation of the model with experimental data given a good agreement results and show that the model is able to predict a correct monomer profile, polymerization rate, particle growth factor and MWD, an algorithm, which embeds physicochemical effects, has been developed to model the industrial reactors.

Keywords Multiscale modeling · Particle growth · Multigrain model · Syndiospecific styrene polymerization · Mass transfer

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Nomenclature

$D_{ef,i}$	Effective macroparticle diffusivity, at the *i*th grid point ($cm^2.\ min^{-1}$)
D_1	Monomer diffusivity in pure polymer ($cm^2.min^{-1}$)
D_s	Effective microparticle diffusion coefficient ($cm^2.\ min^{-1}$)
k_p	Propagation rate constant ($L.\ mol^{-1}\ .hr^{-1}$)
k_d	Catalyst deactivation rate constant (hr^{-1})
k_{tM}	Chain transfer to monomer rate constant ($L.\ mol^{-1}\ .hr^{-1}$)
$k_{t\beta}$	β—hydrogen elimination rate constant (hr^{-1})
k_l	liquid film mass transfer coefficient ($m^2.s^{-1}$)
$M_{M,\ i}$	Monomer concentration in the macroparticle, at the ith grid point ($mol.dm^{-3}$)
$M_{\mu,i}$	Monomer concentration in the microparticle, at the ith grid point ($mol.dm^{-3}$)
M_b	Bulk monomer concentration ($mol.dm^{-3}$)
M_n	Number average molecular weight ($g.mol^{-1}$)
M_w	Weight average molecular weight ($g.mol^{-1}$)
$(mw)_{sty}$	Styrene Molecular weight ($g.mol^{-1}$)
N	Number of shell
r	Radial position at the macroparticle level (m)
r_s	Radial position at the microparticle level (m)
R_c	Radius of catalyst subparticles (m)
R_{N+2}	Macroparticle radius (m)
R_o	Initial particle radius (m)
$R_{h,i}$	Radius of ith hypothetical shells
$R_{s,i}$	Radius of microparticle at ith hypothetical shells
$R_{pv,i}$	Rate of reaction per unit volume at the ith grid point ($mol\ (m^3.s)^{-1}$)
$V_{cs,i}$	Volume of the ith hypothesis shell
$V_{cc,i}$	Volume of catalyst in shell i

Greek Letters

β	Indicator of the monomer convection contribution
λ_{Pk}	kth Moment of live polymers
λ_{Mk}	kth moment of dead polymers