SYSTEM ENGINEERING

非均相催化丙稀聚合的建模与仿真

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摘要　A novel mathematical model for single particle slurry propylene polymerization using heterogeneous Ziegler-Natta catalysts has been developed to describe the kinetic behavior, the molecular weight distribution, the monomer concentration, the degree of polymerization, the polydispersity index (PDI), etc. This model provides a more valid mathematical description by accounting for the monomer diffusion phenomena at two levels as multi-grain model counts, and obtains results that are more applicable to the conditions existing in most polymerizations of industrial interest. Considering that some models on the mesoscale phenomena are so complex that some existing modeling aspects have to be simplified or even
neglected to make the model convenient for use in interesting engi-neering studies, it is very important to put some effort into determining what sort of numerical analysis works best for these problems. For this reason, special attention is paid to these studies to explore an efficient algorithm using adaptive grid-point spacing in a finite-difference technique to figure out more practical mass transport models and convection-diffusion models efficiently. The reasonable outcomes, as well as the significant computation time sav-ing, have been achieved, thereby displaying the advantage of this calculation method.

关键词　modeling and simulation　propylene polymerization　mass transfer　diffusion and convection

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Modeling and simulation of heterogeneous catalyzed propylene polymerization

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Abstract A novel mathematical model for single particle slurry propylene polymerization using heterogeneous Ziegler-Natta catalysts has been developed to describe the kinetic behavior, the molecular weight distribution, the monomer concentration, the degree of polymerization, the polydispersity index (PDI), etc. This model provides a more valid mathematical description by accounting for the monomer diffusion phenomena at two levels as multi-grain model counts, and obtains results that are more applicable to the conditions existing in most polymerizations of industrial interest. Considering that some models on the mesoscale phenomena are so complex that some existing modeling aspects have to be simplified or even neglected to make the model convenient for use in interesting engi-neering studies, it is very important to put some effort into determining what sort of numerical analysis works best for these problems. For this reason, special attention is paid to these studies to explore an efficient algorithm using adaptive grid-point spacing in a finite-difference technique to figure out more practical mass transport models and convection-diffusion models efficiently. The reasonable outcomes, as well as the significant computation time sav-ing, have been achieved, thereby displaying the advantage of this calculation method.

Key words modeling and simulation; propylene polymerization; mass transfer; diffusion and convection

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