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گواهی ثبت مقاله در سیویلیکا
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عنوان مقاله:

Mathematical modeling of the effect of catalyst initialshape and the crack pattern in olefn copolymerization

محل انتشار:

دوفصلنامه پلی اولفین ها, دوره 2, شماره 2 (سال: 1394)

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خلاصه مقاله:

Atwo-dimensional (2D) single particle model for the copolymerization of propylene-ethylene with heterogeneous Ziegler-Natta catalyst is developed. The model accounts for the effects of the initial shape of the catalyst andcarck/ pore patterns on the copolymer composition, polymerization rate and average molecular weight properties.The spherical and oblate ellipsoidal shapes of catalyst particle and four different pattern distributions of cracks andpores in a growing particle are studied in this simulation. It is assumed that the diffusion coeffcient of monomersin the cracks/pores is 10 times higher than that in the compact zone of the particle. In other word, the cracks aredistinguished from the parts with higher monomer diffusion coeffcient. The dynamic 2D monomer diffusionreaction equation is solved together with a two-site catalyst kinetic mechanism using the fnite element method.The simulation results indicate that the initial shape of catalyst changes the average copolymer composition onlyin the early stage of polymerization, but the crack/pore patterns in the growing particle have a strong impact onthe copolymer composition in the polymer particles due to the change of mass transfer limitations. Polyolefns J(2015) 2: 121-133

کلمات کلیدی:

Single particle; Modelling; Finite Element Method; Polyolefn; Copolymerization

لینک ثابت مقاله در پایگاه سیویلیکا:

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