

عنوان مقاله:

Prediction of the Bivariate Molecular Weight and Copolymer Composition Distribution in Free Radical Copolymerization

محل انتشار:

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خلاصه مقاله:

This paper presents the application of an effective method for the calculation of the bivariate molecular weight distribution (MWD) in batch free radical copolymerization of styrene/methyl methacrylate (St/MMA). This method is based on the direct integration of a system of non-linear differential equations describing the conservation of dead polymer and live radicals in a reactor. Probability theory was used to model the microstructure of copolymer chains; specifically an analytical method was used to describe the chemical composition distribution (CCD) and longest monomer sequence length distribution (LSD) of random binary St/MMA copolymer. A fairly general kinetic mechanism was employed to describe the complex kinetics of copolymerization. A comprehensive free-volume model is employed to describe the variation of termination and propagation rate constants as well as the variation of the initiator efficiency with respect to the monomer conversion.

کلمات کلیدی:

Free radical copolymerization; Molecular weight distribution; Chemical composition distribution (CCD); Multicomponent copolymers; Mathematical modeling

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