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Numerical study of copolymer composition and compositional heterogeneity during the synthesis of butadiene-styrene rubber

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Abstract : In the paper the algorithm of modeling of continuous free-radical butadiene-styrene emulsion-type copolymerization process based on the Monte-Carlo method is offered. The analyzed process proceeds in the battery of consistently connected polymerizers (continuous stirred tank reactors) so simulation is carried out taking into account the residence time distribution of particles in the system. The constructed model allows to research molecular-weight and viscous characteristics of the formed copolymer, to predict the weight content of butadiene and styrene in copolymer, to carry out calculation of molecular-weight distribution of the received product and predict copolymer's microheterogeneity at any moment of conducting process.

Keywords: copolymerization, butadiene, styrene, Monte-Carlo method, residence-time distribution, molecular weight distribution, microheterogeneity.

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