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A new approach for mathematical modelling of the dynamic development of particle morphology

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Abstract

A new model for the dynamic evolution of the morphology of polymer-polymer latex particles has been developed. This model overcomes the limitations of the existing methodologies that were only able to provide the morphology of a single particle, which is only a restricted view of the real system that contains a distribution of particle morphologies. Taking into account the relevant kinetic and thermodynamic effects, the new model calculates the distribution of morphologies for the whole population of polymer particles with less computational effort than that needed by the previous models to calculate the morphology of a single particle. The model was validated by fitting the evolution of particle morphology of composite particles during polymerization of methyl methacrylate on a polystyrene seed. Furthermore, the ability of the model to predict the evolution of the particle morphology for different cases was explored.

Keywords: Particle morphology, hybrid particles, (mini)emulsion polymerization

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