

HOW INCREASINGLY POWERFUL PRE MODELING TOOLS ALLOW TO UNLOCK THE FULL POTENTIAL OF FRP AND RDRP IN AQUEOUS EMULSION

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Polymer synthesis in aqueous emulsion *via* free radical polymerization (FRP) and reversible deactivation radical polymerization (RDRP) has been studied extensively for several decades, leading to a detailed fundamental understanding of several underlying kinetic and thermodynamic phenomena.^[1-9] Key has been the development and application of modeling tools. For example, deterministic kinetic modeling tools based on population balances tracking the number of particles containing certain numbers of radical types (Smith-Ewart models) have been widely applied in the past, allowing the identification of important (kinetic) effects such as the segregation and confined space effect. In this presentation, advances regarding both deterministic and stochastic modeling tools are highlighted,^[10-13] considering two main case studies. In a first case study, the application of the most advanced 4-dimensional Smith-Ewart model to date for nitroxide mediated polymerization (NMP) of *n*-butyl acrylate in miniemulsion initiated by MAMA-SG1 is highlighted, demonstrating for the first time the existence of 7 kinetic regimes as a function of the (average) particle size. In a second case study, a bridge is made between deterministic Smith-Ewart and stochastic kinetic Monte Carlo (*k*MCMC) modeling tools. It is specifically illustrated how *k*MCMC allows to track kinetic and thermodynamic information on the level of individual particles. This not only allows to deepen our fundamental understanding of radical polymerizations in emulsion, but also to unlock the full potential of FRP and RDRP in emulsion.

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