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A Mathematical Model for Green Emulsion Polymerization of Methyl Methacrylate in Batch and Semi-Batch Reactors

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Abstract

Emulsion polymerization is a green and sustainable process, as it employs water as the reaction medium, enables high monomer conversion at low viscosity, provides efficient heat removal, and minimizes the use of organic solvents, thereby reducing environmental impact and energy consumption. Owing to lower process temperatures, enhanced heat transfer, and the elimination or significant reduction of volatile organic compounds, emulsion polymerization also contributes to reduced process-related carbon dioxide emissions, supporting pathways toward net-zero carbon manufacturing when coupled with renewable energy sources and solvent-free downstream processing.

In this work, a mathematical model is developed to simulate the isothermal, well-mixed batch and semi-batch emulsion polymerization of methyl methacrylate using a monodisperse particle size approximation. For batch operation, the model predicts the temporal evolution of monomer conversion, rate of polymerization, total particle surface area, and volume-average particle diameter at different initiator concentrations. Model predictions for the total number of particles are compared with experimental data reported in the literature, demonstrating continuous nucleation behavior.

For unseeded semi-batch operation, the effects of monomer feed rate on monomer conversion and particle number are investigated. Good agreement between model predictions and experimental observations is obtained, particularly under monomer-starved operating conditions.

Keywords: Emulsion Polymerization, Methyl Methacrylate, Mathematical Modelling, Batch and Semi-Batch Reactors, Green and Sustainable Processes