557e An Advanced Model for Optimal Operation of Emulsion Terpolymerization Processes: Application to Styrene/Mma/Ma

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A model–based framework for advanced optimal operation of terpolymerization processes was developed. A test case of emulsion terpolymerization of styrene (Sty), methyl methacrylate (MMA) and methyl acrylate (MA) was investigated for predicting and optimising key product properties including molecular weight distribution (MWD), particle size distribution (PSD), terpolymer composition and conversion. The model equations include diffusion-controlled kinetics at high monomer conversions, where transition from a ‘zero-one' to a ‘pseudo-bulk' regime occurs. The reactor mass and energy balances describe the system transients for batch and semi-batch operations. Population balance equations describe the particle evolution and comprise sets of integro-partial differential and nonlinear algebraic equations. The models were solved using an efficient numerical scheme suitable for on-line monitoring and control. The model predictions are experimentally validated in the laboratory and were found to be in excellent agreement, thus paving the way for further application of the model.

Key words: emulsion terpolymerisatin, key product properties, diffusion-controlled kinetics, zero-one, pseudo bulk.