

MODELING OF THE CONCURRENT TANDEM FREE-RADICAL POLYMERIZATION: COPOLYMERS VIA In-SITU MMA TRANSFORMATION FROM THE DEAEMA TRANSESTERIFICATION WITH ETHANOL

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The macroscopic material properties of copolymers are largely affected by microscopic properties such as copolymer composition (the amount of each monomer in the polymer chain) and chain length (number of monomeric units). Copolymers that have used 2-(diethylamino)ethyl methacrylate (DEAEMA) as comonomer are applied in biomedicine, water remediation, CO₂ separation and stabilizers for emulsions and dispersions. A kinetic model is very useful for the prediction of polymer properties and to meet target properties. In the present work, a mathematical model for the FRC of DEAEMA with MMA promoted by transesterification of DEAEMA with methanol based on the continuous variable approximation (CVA) approach is implemented. The numerical solution and fitting of unknown kinetic rate coefficients are implemented in the Matlab software. Five experimental cases are addressed, in which the effect of both initiator (AIBN) and alcohol (CH₃OH) on the monomer conversion, copolymer composition, unreacted monomer concentration and molar mass averages are studied.

Keywords: copolymerization, DEAEMA, modeling

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