

Process optimization by multi-objective Bayesian Optimization of copolymers radical polymerized in a flow synthesizer.

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The properties of polymers are determined by the type of monomers constituting the polymer and by multiple complex factors such as the composition ratio of monomers within the polymer, molecular weight, and molecular weight distribution. Therefore, it is essential that the target values for each of these factors be achieved concurrently. In this study, we employed Multi-objective Bayesian Optimization (MBO) using weighted sums on styrene (St) - methyl methacrylate (MMA) copolymers synthesized via radical polymerization in a flow reactor. We optimized the process so that the composition ratio of monomers within the polymer, monomer conversion, Mw, and Mw/Mn each attained the target values. By the fifth cycle of MBO, it achieved higher weighted sum values than initial points and polymers optimized using Single-task Bayesian Optimization for monomer composition ratio within the polymer. While our MBO approach shows promising capability for the concurrent optimization of multiple objectives, it has not yet identified process conditions that satisfactorily achieve all target values. Future research will explore alternative MBO methods while considering the possibility that the target value may not be appropriate.