Computational Modeling of Dissolution-based Plastic Recycling: Solubility Prediction, Solvent Screening, and Process Design

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ABSTRACT

Dissolution-based plastic recycling is a promising approach to separate and recover high-quality pure polymer resins from plastic waste by exploiting differences in polymer solubility. Recently, we proposed a dissolution-based recycling process, called Solvent-Targeted Recovery and Precipitation (STRAP), in which resins are sequentially recovered from multicomponent plastic waste by selective dissolution followed by precipitation. The design of STRAP processes for complex waste streams with several components requires careful consideration of solvent selection, operating temperatures, and the sequence of dissolution/precipitation steps. Determining these choices is challenging due to the wide range of solvents and temperatures that could be possibly used for a given set of target polymers. Here, we report a computational scheme to predict polymer solubilities and design STRAP processes. We first employed molecular dynamics simulations and the conductor-like screening model for real solvents to predict temperature-dependent polymer solubilities in various solvent systems. With this approach, we established a computational solubility database for over 10 common polymers in 1007 solvents at multiple temperatures. Solubilities were experimentally measured in selected systems to validate computational predictions. We then developed a tool that automates the selection of solvents for all possible polymer dissolution sequences to identify feasible STRAP processes. We show that this tool can be combined with process simulation models to study the economic and environmental impact of different dissolution/precipitation sequences. Finally, we demonstrate the application of these computational methods via multiple case studies in which pure resins are successfully recovered from polymer mixtures, indicating the capability of using computational tools to guide effective STRAP process design.