Abstract

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Designing configurations for multicomponent distillation, a ubiquitous process in chemical and petrochemical industries, is often challenging. This is because, as the number of components increases, the number of admissible distillation configurations grows rapidly and these configurations vary substantially in their energy needs. Consequently, if a method could identify a few energy-efficient choices from this large set of alternatives, it would be extremely attractive to process designers. Towards this, we develop the first mixed-integer nonlinear programming (MINLP) based solution approach that successfully identifies the most energy-efficient distillation configuration for a given separation. Current sequence design strategies are largely heuristic. The rigorous approach presented here can help reduce the significant energy consumption and consequent greenhouse gas emissions by separation processes.

In addition to the combinatorial complexity, the challenge in solving this problem arises from the nonconvex fractional terms contained in the governing equations. We make several advances to enable solution of these problems.

1. We propose a novel search space formulation by embedding convex hulls of various important substructures. We prove that the resulting formulation dominates all the prior formulations in the literature.

2. We derive valid cuts to the problem by exploiting the monotonic nature of the governing equations.

3. We adapt the classical Reformulation-Linearization Technique (RLT) for fractional terms. Our RLT variant exploits the underlying mathematical structure of the governing equation, and yields a provably tighter convex relaxation.

4. We construct the simultaneous hull of multiple nonlinear terms that are constrained over a polytope obtained by intersecting a hypercube with mass balance constraints. This yields a tighter convex relaxation than the conventional approach where the nonlinear terms are convexified individually over a box.

5. A key challenge in constructing a valid convex relaxation has been that the denominator of certain fractions in the governing equation can approach arbitrarily close to zero. Using our RLT variant, we construct the first valid relaxation.

6. We leverage powerful mixed-integer programming (MIP) solvers by implementing a discretization-based solution procedure with an adaptive partitioning scheme.

With extensive computational experiments, we demonstrate that the proposed approach outperforms the state-of-the-art in the literature. The formulation can be tailored to other objectives by appending the relevant constraints. Here, we present an extension that identifies the distillation configuration that has the highest thermodynamic efficiency. Finally, we illustrate the practicality of the developed approaches with case studies on crude fractionation and natural gas liquid recovery.