

Advances in Modelling and Optimization of Multicomponent Distillation Configurations

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Accounting for 90-95% of liquid phase separations, distillation is ubiquitous in chemical and petrochemical industries, separating mixtures such as crude petroleum, natural gas liquids, air, and alcohols. It is also estimated to account for 2.5% of the total energy used in the U.S.A. Therefore, reducing the energy consumption of distillation, the motivation for this thesis, is an important endeavor to not only save on operating costs in chemical plants but also cut down greenhouse gas emissions.

One manner of energy reductions is identifying new alternative designs for distillation which are more energy-efficient than the current practice. While well-established commercial process simulators exist for evaluating distillation, design features such as sloppy splits and thermal couplings (which are valuable for energy savings) not only make these evaluations computationally challenging (for both feasible solutions and optimization), but also result in a combinatorial explosion of the search space. For example, there are 6,128 different distillation configurations possible for separating a five-component mixture. To overcome this hurdle, we use shortcut models, which capture the essential physics of the separation, to reliably screen through the vast search space of configurations, in order to quickly identify a handful of candidates which can be subsequently analyzed in a process simulator.

Two common assumptions in shortcut models for distillation are constant relative volatilities and constant molar overflow. These have been invaluable in the past to not only dramatically reduce the computational complexity of evaluating distillation, but also enable the derivation of generalizable insights and constraints which would be unfathomable with detailed models. However, their usage has also been censured for not holding up in the physics of the real world. To address this, we developed a parameter estimation method for relative volatilities and employed a simply variable transformation to relax the constant molar overflow assumption in our shortcut model. These techniques have the combined advantage of expanding the applicability of these assumptions while retaining the mathematical simplicity, and thereby computational tractability, granted by them.

Heat integration is important during the search for energy-efficient configurations, as it can bring about substantial energy savings. However, ascertaining the feasibility of proposed heat integrations have hampered global optimization in the past, as traditional checks calculate temperatures by complex equations. We developed a new metric, pseudo relative volatility, and used it to build a shortcut criterion which is computationally cheaper to check for feasibility. After implementing this, our optimization formulation is now capable of identifying heat-integrated and energy-efficient configurations for distillation.

A fundamental reason why distillation can be used as a separations technology is that components are separated on the basis of their volatility: lighter components are recovered more in the distillate product than the bottoms. While this behavior is common knowledge, we developed the first proof that a mathematical model of distillation can guarantee it. Furthermore, we derived a new stronger relation which bounds component recoveries in multicomponent distillation.

With these advances, we can now search the vast space of multicomponent configurations to more reliably identify energy-efficient and heat-integrated configurations, and our methodology has been successfully applied on an important and challenging industrial separation.