Advances in the Design of Heat Integrated & Heat Pump Assisted Distillation Systems

Akash Sanjay Nogaja

The push for lower green house gas emissions, coupled with the direct availability of carbon free electricity has incentivized the chemical and refining industry towards electrification of unit operations. Among these, the prime candidates are the distillation systems which are used for purifying mixtures and are responsible for an estimated 6-10% of industrial energy in the US. Electrifying such systems hold significant potential for reducing carbon emissions. However, directly converting carbon-free electricity into heat for vaporizing liquid in the reboiler is an impractical approach, as it would demand disproportionately large renewable energy installations. Instead, heat pumps, which transfer heat from a low-temperature source (the condenser) to a high-temperature sink (the reboiler) using only a fraction of the energy compared to the amount of heat transferred, offer a more viable and energy-efficient alternative for integration with renewable energy sources.

Despite their advantages, heat pumps have seen limited adoption in above-ambient temperature applications. This is largely due to the historically low cost of fossil fuels and the high capital investment associated with compressors in heat pump loops. While strategies such as intermediate reboilers and condensers have been proposed to reduce the power requirements of heat pump systems, these approaches often require multiple compressors, further increasing capital costs. In this research, novel insights are presented into the use of multi-effect systems in binary distillation that replicate the energy savings of intermediate heat exchangers, while requiring only a single compressor, offering a more cost-effective and energy-efficient alternative. The concept of 'Separation Cogeneration' is introduced that recovers a significant fraction of the electrical energy supplied to the compressors as useful heat, thereby, further boosting the first and second law efficiencies.

Additionally, most industrial separations involve multicomponent mixtures. The number of possible configurations (alternative process pathways that achieve the same separation) grow combinatorially with the number of components. These configurations can differ significantly in energy demand. Evaluating each configuration using commercial process simulators is computationally prohibitive, and practitioners relying on heuristics to design distillation sequences and then operating them using heat pumps may often select suboptimal designs with unnecessarily high energy requirements.

In this research, the aforementioned challenges are addressed through the following key contri-

butions:

1. Enhancing the energy efficiency of multicomponent distillation systems by enabling heat integration between condensers and reboilers through pressure manipulation of individual columns.
2. Developing a computationally tractable and accurate surrogate model for temperature prediction and heat pump work estimation, suitable for integration within global optimization frameworks.
3. Formulating optimization models capable of identifying globally optimal configurations that minimize total energy consumption while adhering to practical limits on the number of compressors used.

The temperature surrogate model was developed by integrating the Antoine equation with the assumption of constant relative volatility. This model effectively captures the non-linear temperature profiles of phase-changing multicomponent mixtures, achieving an accuracy of $R^2 \approx 0.99$.

Additionally, while exergy loss has traditionally been used as a proxy for heat pump work in distillation literature, this study clearly delineates the conditions under which that approximation is valid. To address its limitations, we introduce the concept of 'Minimum Heat Pump Work', a more accurate proxy for actual compressor work and establish a tighter theoretical lower bound for the energy required by a heat pump. These insights form the basis for the development of the proposed surrogate heat pump model.

The case studies presented in this research reaffirm that heuristic methods or sequential optimization approaches may overlook promising, non-conventional configurations that are both financially viable and capable of significantly reducing carbon emissions.