Optimal Design of Heat Pump Assisted Distillation Sequences

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Abstract

This study demonstrates enhanced distillation sequence efficiency achieved through the simultaneous optimization of column sequences and various heat integration methods, including thermal couples, direct integration (reboiler-condenser heat exchange), and assisted integration via vapor recompression and bottom flashing cycles. The model applied to the separation of a 4-hydrocarbon mixture, reveals a substantial reduction in total utility costs (hot, cold, and electricity) compared to the top-performing non-heat integrated alternative (fully thermally coupled distillation sequence), achieving a remarkable 78% reduction.

In alignment with the "Roadmap to Achieve Net Zero Emissions by 2050," the proposal to electrify distillation sequences is introduced to replace non-renewable utilities with electricity. Despite cost increases, the optimal electrified solution remains competitive with the best non-heat integrated alternative. However, in sequences involving challenging separations, the most effective solution may necessitate electricity as the sole utility.**Keywords**: Distillation, Vapor Recompression, Electrification, Bottom Flashing, Heat Integration.

* 1. Introduction

Energy consumption in the industrial sector constitutes approximately one-third of the global energy used, reaching 156 EJ (1.56 1020J) in 2020 and is projected to reach 207 EJ in 2050 (IEA, 2022). Within this sector, chemical and petrochemical industries account for 20-30%. For example, the European Union recorded 21.5% in 2021 (Eurostat), which is around 2.159 EJ. Distillation is the predominant method used for approximately 90 to 95% of all separations and purification processes. This means that distillation contributes to around 40-60% of the energy consumption in chemical and petrochemical industries (Sholl & Lively, 2016).

There are many alternatives to increase the energy efficiency of distillation, such as direct heat integration, thermally coupled distillation (TCD), heat pump-assisted distillation, and multi-effect distillation, etc. (Kruber et al., 2021). Although, ongoing advancements in distillation yield substantial energy and cost savings, fossil fuels remain the primary energy source for distillation.

However, a transformative shift is currently underway, as highlighted in the "Roadmap to Achieve Net Zero Emissions by 2050" (NZE scenario) (IEA, 2022). In this NZE scenario, electricity is set to play a central role in the global energy landscape, with renewables growing fourfold by 2030. Key milestones include 50% low-emission electricity by 2025, advanced economies' electricity sector achieving net-zero emissions by 2035, and 40% of industrial energy being electric by 2040. The plan aims for 50% of heat demand met by heat pumps by 2045 and 90% renewable-sourced electric energy by 2050, aligning with Industry 4.0's goal of transitioning from fuel to electrified processes.

In this work, we present a comprehensive superstructure for generating optimal distillation sequences that simultaneously considers all the possible heat integration alternatives such as thermal couples, direct condenser-reboiler heat integration, and vapor recompression/bottom flashing between different condenser/reboilers not necessarily in the same column.

The objectives are twofold. Firstly, we strive to minimize the overall cost associated with the distillation process. Simultaneously, we aim to maximize the utilization of electricity. We demonstrate that, in certain scenarios, these objectives are not conflicting; however, a substantial compression cost may result in an excess cost for the electrification process.

* 1. Synthesis of heat pump assisted distillation sequences.

The problem we are dealing with can be stated as follows. Given is a zeotropic N component mixture, we want to separate the individual components using distillation columns considering simultaneously the possibility of thermal couples, direct heat integration (e.g. reboiler-condenser heat exchange), and indirect heat integration through vapor recompression of the vapor before entering the condenser or bottom flashing of the liquid previous to the reboiler. The objective is twofold, to minimize the total annual cost and to significantly decrease the reliance on hot utilities derived from fossil fuels, effectively electrifying the chemical industry.

The initial phase involves the creation of a comprehensive superstructure encompassing all relevant alternatives. For this purpose, we utilize a superstructure exhibiting intermediate characteristics bridging the gap between the State Task Network and State Equipment Network formalism (Yeomans & Grossmann, 1999). The generation process is as follows:

* First, we generate all the possible sub-mixtures (States) excluding final products. For example, in a 4-component mixture, these are ABCD, ABC, BCD, AB, BC, and CD (components named with capital letters ordered by decreasing relative volatilities). For each state, we then generate all potential separation tasks. For instance, for the initial ABCD mixture, tasks include A/BCD, AB/BCD, AB/CD, ABC/BCD, ABC/CD, and ABC/D. Each separation task can be conceptualized as a "pseudo-column," comprising rectifying and stripping sections where components to the left of the slash move to the distillate, those to the right go to the bottoms, and those on both sides are optimally distributed between distillate and bottoms. For instance, in the ABC/CD separation, B is the light key, D is the heavy key, and C is distributed between the distillate and bottom streams. It is important to note that when the sequence of states is fixed, the sequence of separation tasks is entirely determined.
* According to Caballero & Grossmann (2006) and Giridhar & Agrawal (2010), the search space must be formed by ‘regular configurations’ (sequences of tasks/ states that can be reordered in exactly N-1 columns). So, we must include a set of logical relationships that ensure only regular configurations. See Caballero & Grossmann (2006) for a comprehensive discussion on this topic.
* The connection between two different states can be through a thermal couple, a condenser (reboiler), a vapor recompression (VR) at the top of a column, or a Bottom Flashing (BF). (See Figure 1a, 1b)
* In the case in which two separation tasks generate the same state, these two columns can be stacked to form a single column. In general, it is necessary to increase the reflux (or boil-up) in one of those columns to compensate for the imbalance in flows in the connection. Alternatively, it is possible to use a condenser/reboiler at that point to compensate for the flow imbalance (Caballero & Grossmann, 2014). This second approach has the advantage of increasing the possibilities for heat integration (Navarro et al., 2013) and it is the approach followed in this work. (See Figure 1c)

To promote direct heat integration, we must allow the distillation columns to operate at different pressures (and therefore different temperatures in the condenser and reboiler). But there are some constraints. Two columns connected by a thermal couple, or two stacked columns must be at the same nominal pressure. Besides, to avoid very different diameters in different sections of the columns all the streams entering a distillation column are assumed to be saturated liquid.



Figure 1. Alternatives for the connectivity between columns. a) The rectifying section of a task includes a condenser (small dotted line, in green), a thermal couple (dotted magenta lines), and Vapor Recompression (continuous lines in blue). b) Stripping section: reboiler (small dotted line in orange, thermal couple (dotted magenta lines), and Bottom Flashing (continuous line in red). c) Stripping and rectifying section sharing a common state.

Heat integration encompasses all the condensers, reboilers, coolers in VR, heaters in BF, as well as all heaters/coolers required to obtain saturated liquid in the feed points to columns and to address the vapor/liquid imbalance in stacked columns. Heat integration is simultaneously optimized with the operating conditions of the rest of the system (separation sequence, column pressures, pressure change in compressors, etc.) using pinch analysis (Duran and Grossmann, 1986)

* 1. Case Study

To exemplify the capacities of the proposed approach we examine the separation of an equimolar mixture of 4 hydrocarbons (n-pentane, n-hexane, n-heptane, n-octane). Table 1 presents the data for the example.

The distillation columns were simulated using the Fenske-Underwood-Gilliland (FUG) shortcut. The relative volatilities exhibit some pressure dependence and were computed rigorously using the Peng Robinson equation of state at the conditions of the feed at each column, employing Aspen-HYSYSTM as a thermodynamic properties server. The rest of the operations including compressors and valves in vapor recompression and bottom flashing cycles, pumps, and all heat transfer operations (condensers, reboilers, and feed conditioning) were also rigorously calculated using Aspen-HYSYSTM as a thermodynamic server.

The optimization includes the cost of energy, the main equipment (columns, compressors, compressor drivers, and pumps), and an estimation of the heat transfer equipment assuming a vertical heat transfer approach. (Smith, 2016) However, the actual structure of the heat exchanger network is calculated a posteriori using a sequential approach (Biegler et al., 1997).

Table 1. Data for the example.

|  |  |  |  |
| --- | --- | --- | --- |
| **Components** | Composition(mol fraction) |  |  |
| n-pentane | 0.25 | Feed Flow  | 200 kmol/h  |
| n-hexane | 0.25 | Feed Pressure  | 100 kPa |
| n-heptane | 0.25 | Feed Temperature | 25 ºC |
| n-octane | 0.25 |  |  |
| **Cold Utilities** | Cost ($/kW·y) | **Hot Utilities** | Cost ($/kW·y) |
| Water  | 10.19 | HP Steam | 509.76 |
|  Electricity 800 $/kW·y  |
|  Interest = 10% in 10 years  |
|  Cost estimation based on correlations by (Turton et al., 2018) Thermodynamics Peng Robinson (default Aspen-HYSYS parameters) ΔTmin in Heat Exchanger Network: 10 ºC Isentropic Efficiency in compressors: 75% Nominal Pressure in columns between [100 – 1000] kPa Minimum pressure after a valve: 10 kPa |

The optimal separation sequence consists of a set of separation tasks, where the light and heavy key components are determined by their extreme volatilities (ABC/BCD - AB/BC – BC-CD – A/B – B/C – C/D) but unlike what might be expected if all columns were maintained at the same nominal pressure, in which we would get a fully (or almost) thermally coupled configuration, the optimal solution takes advantage of a large number of heat integration opportunities, Notably, only a thermal couple connects the bottoms of separation ABC/BCD with the feed of separation BC/CD. Additionally, a VR cycle emerges, replacing the condenser in the separation task AB/BC.

The existence of a Thermal Couple allows us to go a step further and reduce by one the total columns by introducing an internal wall. Figure 2(a) shows the optimal configuration using three distillation columns. Figure 2(b) shows the intensified counterpart and Figure 2(c) shows the heat exchanger network.

The total annualized cost of the best solution is $1.235 106 per year, with approximately 61% attributed to operating costs (mainly utilities). For the sake of comparison, the total cost of hot utilities in the fully thermally coupled configuration is $1.337 106/y. that is 77% more than the total utilities in the proposed solution.

Adhering to the recommendations outlined in the «Roadmap to Achieve Net Zero Emissions by 2050» which advocates for electrifying the chemical industry, it becomes possible to identify an optimal sequence where hot utilities are not employed (not presented due to space constraints). In this scenario, the total annualized cost rises to $1.721·106/y, an increase of approximately 39%, but remains competitive with the best non-heat integrated sequence.

It is worth remarking, that difficult separations tend to favor the presence of VR / BF configurations because the difference in temperatures is relatively small and therefore the compression work is also reduced. In those cases, it is even possible that the best configuration does not include non-renewable utilities.





Figure 2. Best solution obtained. a) Regular configuration (N-1 columns) A: n-pentane, B: n-hexane, C: n-heptane, D: n-octane. In square brackets is a code to identify the streams in the Heat Exchanger Network. b) Thermodynamically equivalent intensify sequence. Columns 1 and 2 are merged in a Divided Wall Column. c) Heat Exchanger Network.

* 1. Conclusions

In this work, we have shown that it is possible to increase the efficiency of distillation sequences by concurrently optimizing the column sequence and exploring various heat integration alternatives, such as, thermal couples, direct integration (reboiler–condenser heat exchange), and assisted heat integration by the use of vapor recompression cycles using the vapor from the top of the separation sequences and bottom flashing by expanding the liquid before entering the reboiler.

The model was exemplified through the separation of a 4-hydrocarbon mixture, showcasing a significant reduction in total utility costs (encompassing hot, cold, and electricity) compared to the most effective non-heat integrated alternative—a fully thermally coupled distillation sequence. For the presented example, this reduction reached an impressive 78%.

In the spirit of the "Roadmap to Achieve Net Zero Emissions by 2050" electrifying the distillation sequence is proposed to eliminate the use of non-renewable utilities, substituting them with electricity. Despite the associated cost increase, the optimal solution remains competitive with the best non-heat integrated alternative. However, this is not necessarily always the case. In sequences with some difficult separations, the best result might include electricity as the sole utility.

Acknowledgments

The authors acknowledge financial support from the «Ministerio de Ciencia e Innovación», Spain, under project PID2021-124139NB-C21, and to the «Conselleria de Innovacion, Universidades, Ciencia y Sociedad Digital of the Generalitat Valenciana», Spain, under project PROMETEO/2020/064.

References

Biegler, T.L., Grosmmann, I.E., Westerberg, A.W., 1997. Systematic Methods of Chemical Process Design. Prentice Hall PTR., Upper Saddle River, NJ. USA.

Caballero, J.A., Grossmann, I.E., 2006. Structural Considerations and Modeling in the Synthesis of Heat-Integrated−Thermally Coupled Distillation Sequences. Ind. Eng. Chem. Res. 45, 8454–8474.

Caballero, J.A., Grossmann, I.E., 2014. Optimal synthesis of thermally coupled distillation sequences using a novel MILP approach. Comput. Chem. Eng. 61, 118–135.

Duran, M.A., Grossmann, I.E., 1986. Simultaneous optimization and heat integration of chemical processes. AIChE J. 32, 123–138.

Giridhar, A., Agrawal, R., 2010. Synthesis of distillation configurations: I. Characteristics of a good search space. Comput. Chem. Eng. 34, 73.

International Energy Agency (IEA)., 2022. World Energy Outlook. https://www.iea.org/reports/world-energy-outlook-2022

Kruber, K.F., Grüters, T., Skiborowski, M., 2021. Advanced hybrid optimization methods for the design of complex separation processes. Comput. Chem. Eng. 107257.

Navarro-Amorós, M.A., Ruiz-Femenia, R., Caballero, J.A., 2013. A new technique for recovering energy in thermally coupled distillation using vapor recompression cycles. Aiche J. 59, 3767–3781.

Sholl, D.S., Lively, R.P., 2016. Seven chemical separations to change the world. Nature 532, 435–437. https://doi.org/10.1038/532435a

Smith, R., 2016. Chemical Process Design and Integration, 2nd edition, John Wiley & Sons. West Sussex, United Kingdom.

Turton, R., Shaeiwitz, J.A., Bhattacharyya, D., Whiting, W.B., 2018. Analysis, Synthesis, and Design of Chemical Processes. 5th edition. Prentice Hall.

Yeomans, H., Grossmann, I.E., 1999. A systematic modeling framework of superstructure optimization in process synthesis. Comput. Chem. Eng. 23, 709–731.