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Pimp my Distillation Sequence – Shortcut-based Screening of Intensified Configurations

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ABSTRACT

Distillation processes account for a substantial share of the industrial energy demand. Yet, these energy requirements can be reduced by a variety of energy integration methods, including various forms of direct heat integration, multi-effect distillation, thermal coupling and vapor recompression. Consequently, these intensification methods should be evaluated quantitatively in comparison to each other for individual separation tasks, instead of benchmarking single options with conventional sequences or relying on simplified heuristics. In order to overcome the computational burden of a broad assessment of a large number of process alternatives, a computationally-efficient framework for the energetic and economic evaluation of such energy integrated distillation processes is presented, which builds on thermodynamically-sound shortcut models that do not rely on constant relative volatility and constant molar overflow assumptions.

Keywords: Distillation, Energy Integration, Shortcut Screening, Thermal Coupling, Heat Integration

1. INTRODUCTION

To mitigate climate change effectively, we must reduce the energy requirement and greenhouse gas emissions in the chemical industry, which is one of the largest sources of global industrial greenhouse gas emissions [1]. The majority of these emissions result from energy requirements that are to a large extent caused by thermal separations, where distillation processes remain dominant [2]. While other separation processes are beneficial for certain applications, theoretical studies have shown that these technologies do not easily outperform distillation even under ideal conditions [3]. Numerous energy integration techniques have been developed to enhance the energy efficiency of distillation processes [4], especially for the separation of multi-component mixtures that typically require distillation column sequences.

For direct heat integration, the pressure in at least one column is adjusted such that the heat-supplying column's top temperature is higher than the heat-receiving column's bottom temperature to allow rejected heat from one column to drive the reboiler of another [5]. When both columns have similar duties, direct heat integration can reduce the energy demand by up to 50%.

Multi-effect distillation extends the concept of direct heat integration by e.g. dividing the feed stream among multiple columns conducting the same separation at different pressures. If a binary separation is performed by two (three) such integrated columns, this is also referred to as dual (triple) effect distillation. The net energy demand of multi-effect sequences is approximately that of the conventional separation divided by the number of utilized effects, offering substantial energy-saving potential at the cost of increased investment for a larger number of columns.

For thermal coupling, heat exchangers and liquid streams between adjacent distillation columns are replaced by bidirectional liquid and vapor transfer, effectively combining energy and mass integration [6]. Thermal coupling and the equipment-integrated dividing wall column (DWC), which combines multiple separations in a single column shell, are considered among the most prominent examples of process intensification in fluid separations, also lowering capital costs by around 30% compared to non-integrated distillation processes [7].

These concepts compete with heat-pump assisted distillation for upgrading and integration of rejected heat, such as mechanical vapor recompression (VRC) which uses the overhead vapor as the working fluid in an open Clausius-Rankine cycle [8]. Other approaches include

closed-cycle heat pumps with freely selectable working fluids [9] and less commonly used concepts like internally heat-integrated distillation columns (HIDiC), which has proven inferior to VRC [10, 11]. Heat pumps require the use of expensive compressors, but have the potential to transform a thermally-driven process into an electrically-driven while improving the energy efficiency significantly [12].

While all of these concepts may enable significant energy savings in respect to conventional distillation sequences, few studies compare alternative approaches that may offer similar benefits. Additionally, the combination of multiple energy-integration concepts, such as thermal coupling and VRC [13], is rarely explored on a broader basis, yet it can significantly increase the potential for energy savings, as well as the number of possible flowsheets.

It is important to note that the actual savings and best flowsheet options depend heavily on the specific separation task, necessitating case-specific evaluations that cannot be adequately addressed with heuristics. Therefore, a quantitative comparison of a broad range of energy integration concepts is crucial to accurately assess their savings potential and identify the flowsheets of highest interest for a specific separation task, as e.g. illustrated by Cui *et al.* [14] for few selected Multi-effect and VRC configurations.

Many methodologies have been developed to identify energy-efficient distillation flowsheets. Especially Agrawal and co-workers have presented elaborate synthesis approaches to generate conventional and thermally coupled configurations [15–17], applying global optimization on the basis of the Underwood equations to evaluate vapor duty [18], exergy losses [19], or total annualized cost (TAC) [20]. Complementary strategies combine shortcut evaluations and metaheuristic optimization to explore various integration concepts, including heat integration and VRC [21–23]. However, all of these approaches rely on the Underwood equations, which build on constant molar overflow (CMO) and constant relative volatility (CRV), limiting the applicability to non-ideal mixtures.

Although rigorous simulation-based approaches [24, 25] effectively handle non-idealities, they are computationally intensive, making such evaluations time consuming [26].

Brüggemann and Marquardt [27] first applied a shortcut-based approach based on rigorous thermodynamics for screening a limited number of conventional and thermally coupled sequences, which was further extended by Skiborowski [28] to cover direct heat integration, as well as multi-effect distillation and some direct combinations with VRC. The current contribution extends this approach further by enabling all possible VRC configurations for an extended set of simple and (heat integrated) thermally-coupled sequences resulting in a total of 773 process alternatives.

To further address that the different configurations require different equipment, including expensive compressors, the thermodynamically sound evaluation of the minimum energy demand (MED) is extended by a capital cost estimation, in order to facilitate a multi-objective evaluation of different process configurations in terms of net energy demand, operating cost, capital investment, and TAC estimates. The capabilities are demonstrated for the well-known separation of benzene, toluene and p-xylene, illustrating the applicability for rapid decision making. Note, that the current study does not cover thermally-coupled sequences without vapor transfer [29], which can provide further potential for heat integration [30] and extend the design space.

2. SHORTCUT SCREENING FRAMEWORK

The algorithmic framework for the automatic evaluation of energy-integrated distillation processes is presented in Figure 1. Thermodynamic property data for a given chemical system is provided is the form of a text file and can be extracted from e.g. Aspen Plus using a report file parser. The screening tool in the centre of the framework, which is implemented in MATLAB, implements all considered process alternatives for the separation of a multicomponent mixture into three products and automatically determines all relevant mass and energy streams, temperatures, pressures as well as their energy demand and economic performance. A result explorer enables a graphical performance evaluation for rapid decision making.
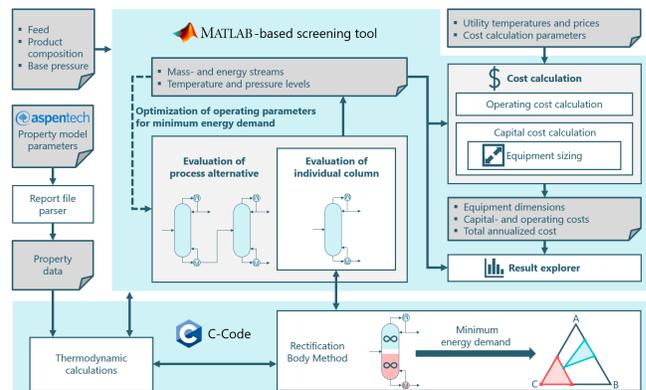

Figure 1: Schematic of algorithmic framework for fast evaluation of energy-integrated distillation processes

2.1 Implemented process configurations

The following subsections summarize the covered process alternatives for the separation of a multicomponent feed stream into three product fractions.

2.1.1 Simple column configurations

The three simple sequences of conventional columns for ternary separation problems include the direct and indirect sequence, which both have two columns, and the sloppy split, which eliminates one of the products from each of the first column's product streams and consists of three columns.

2.1.2 Thermally coupled configurations

Six thermally coupled configurations can be derived from the simple sequences, based on the decomposition approach proposed by Carlberg and Westerberg (1989) [31]. These include a side rectifier, a side stripper and 4 prefractionator configurations, considering no, partial or full thermal coupling (equivalent to Petlyuk-configuration) between the prefractionator and the main column. In practice, thermal coupling requires bidirectional transfer of liquid and vapor between the coupled columns, which is approximated by superheating or subcooling of the intermediate product streams [32].

2.1.3 Directly heat integrated configurations

The previously shown sequences with two or more hydrodynamically decoupled columns can benefit from direct heat integration. For this, the pressure in at least one of the columns needs to be adjusted, such that the top temperature of the heat supplying column is higher than the bottoms temperature of the heat receiving column. The necessary operating pressure of the columns is determined by means of flash calculations for a fixed approach temperature of 10 K, avoiding a complex economic optimization. Additional heat exchangers consider the heat required to keep the feed at liquid boiling conditions at altered column pressures and any additional heating or cooling duty required to compensate for mismatched condenser and reboiler duty of the heat-integrated columns.

Each condenser of one column can act as the heat source, while each reboiler of another column can act as the heat sink, and either the pressure in the heat supplying column is increased or the pressure in the heat receiving column is decreased, leading to four combinations each for conventional sequences and the prefractionator with two columns. For the sloppy split with three columns, 30 possible combinations can be derived, including columns that act as the heat receiving column for another column, while simultaneously supplying heat to the remaining column. In this form a total of 42 configurations with direct heat integration are considered.

2.1.4 Multi-effect distillation

Multi-effect distillation applies direct heat integration between two columns conducting the same separation at different pressures by dividing the feed stream

between multiple columns. The working pressure is determined identically as for directly heat integrated sequences and the feed stream is distributed such that the columns are integrated without remaining duty. In total, 13 dual-effect and 13 triple-effect variants are evaluated for the three simple column configurations, considering multi-effect distillation for each individual column as well as any combination of columns.

2.1.5 Vapor recompression

The flowsheet and open compression cycle for an individual column with vapor recompression are shown in Figure 2. The high pressure level is determined via flash calculations such that the dew temperature of the pressurized vapor is 5 K higher than the saturation temperature of the heat receiving stream. The electrical compressor duty is determined based on an isentropic compression with an isentropic efficiency of 85 % and mechanical efficiency of 95 %. Superheating of the vapor before compression to avoid condensation in the compressor and additional heat exchangers for remaining heat requirements are considered. For any of the previously presented sequences, vapor recompression between each combination of condenser and reboiler is considered, resulting in almost 700 different VRC configurations, which also combine heat pumps with other energy integration methods.
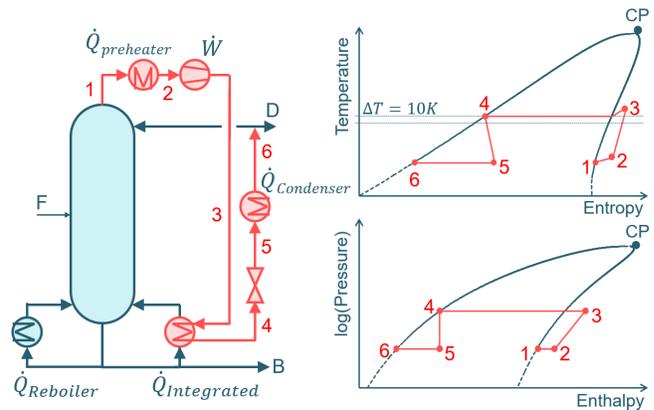

Figure 2: Flowsheet and compression cycle diagrams of VRC for individual column

2.2 Minimum energy demand calculation

The MED of individual splits is calculated with the Rectification Body Method (RBM) [33], building on the process synthesis software collection of AVT.SVT at RWTH Aachen[1] . The RBM is a thermodynamically sound pinch-based shortcut, which only assumes an infinite number of equilibrium stages and accordingly separation to the highest achievable purity along isobaric operation. The MED is computed based on the intersection of the

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rectification bodies of the stripping and rectifying sections, assuming that this enables a continuous stage-to-stage profile that renders the separation feasible. Refer to Skiborowski *et al.* [34] for a more detailed overview on pinch-based shortcut methods.

The energy demand of a configuration is determined as the net sum of all externally supplied heat and electricity. For sloppy splits and all derived configurations, including all prefractionator and heat integrated configurations, the distribution of the intermediate product fraction in the first column affects the energy demand of the configuration and is thus determined by means of a gradient-based local optimization of the net energy demand of the entire configuration, which determines the flowrates and compositions of the internal streams.

2.3 Operating and capital cost calculation

The economic evaluation is performed based on the operating cost and capital cost estimations derived from the MED computations, which are combined into total annual cost with an interest rate of 6% and a depreciation period of 10 years. For this evaluation, the operating costs are determined based on the utility requirements with temperatures and costs for utilities and electricity are considered according to the values in the book of Turton *et al.* [35]. For each heat exchanger the cheapest available utility resulting in a temperature difference of 10 K in the heat exchanger is selected.

The capital costs of each piece of equipment are calculated with Guthrie's module factor method [36] following an equipment size estimation, applying the Winn equation to calculate the minimum number of stages and the Gilliland correlation [37] with an approximation for actual reflux ratio $r = r_{min} \cdot 1.2$, based on the minimum reflux ratio r_{min} determined with RBM. The actual number of stages is finally obtained as the next highest integer while also considering the tray efficiency. The column and tray stack height are calculated according to Douglas [37, p. 453] based on actual number of stages tray spacing, which also determines the flooding factor.

The diameter of each column is calculated using the approach of Douglas [37] which builds on the estimation of the volumetric vapor flow rate on the basis of the boilup vapor stream. The heat exchanger area is calculated with the respective duty, specified U-value and (logarithmic) mean temperature difference. The costs of VRC are considered with the additional capital investment for the compressor according to Biegler *et al.* [36] and electricity demand for operation, while the demand for hot and cold utilities is reduced.

3. CASE STUDIES

To illustrate the applicability and capabilities of the algorithmic framework, a liquid boiling feed stream of 10 mol/s consisting of an equimolar mixture of the well studied mixture of benzene, toluene and p-xylene [38] is separated into pure products at a reference pressure of 1 atm. The vapor liquid equilibrium is calculated using NRTL as activity coefficient model, Redlich-Kwong as equation of state for the vapor phase, the extended Antoine equation, as well as DIPPR correlations for the specific heat capacities and heat of vaporization.

The screening of all 774 process options requires about 10 min on a PC with an Intel i7-8700 CPU using MATLAB R2024b. Considering only configurations for which the temperature levels of the chosen utilities are suitable for external heating and cooling, 60 configurations with larger pressure variations are discarded. Limiting the scope further to processes with column pressures above 100 mbar, a maximum compression ratio of 7 for VRC configurations and a maximum compressor discharge temperature of 150 °C, 196 variants remain, while many of the VRC variants are excluded because the boiling point of p-xylene (138 °C) is very close to the discharge temperature limit.

Of the ten sequences with the lowest net energy demand, nine utilize VRC while a variant of the prefractionator with heat integration from the first to the second column (PF-HI12) ranks #6 (MED = 237.3 kW) and takes position #4 regrading TAC (221.5 k$). The lowest net energy demand (MED = 161.6 kW) is determined for a direct sequence with VRC for each column, ranking third regarding TAC (214.8 k$).

Of the ten sequences with the lowest TAC, four utilize only VRC, four only direct heat integration and the remaining processes combine direct heat integration with either thermal coupling or VRC, indicating that both means for heat integration are economically competitive in the current scenario. A direct sequence with direct heat integration from the first to the second column (DS-HI12) has the lowest TAC (207.0 k$) and also ranks #22 regarding MED (259.7 kW). The non-integrated direct sequence is the best performing simple sequence, but only ranks #191 regarding MED (627.5 kW) and #145 for TAC (325.4 k$), so the best sequences have 74.2% lower MED and 36.4% lower TAC respectively. The fully thermally coupled DWC only ranks #115 regarding net MED (435.1 kW) but considering capital savings by construction with a single column shell it ranks #13 regarding TAC (249.1 k$).

The best 20 processes regarding TAC are highlighted in Figure 3, summarizing the TAC distribution for all practically feasible sequences. All sequences requiring electricity use VRC effectively limiting operating costs, but require significant investment for the compressors. Interestingly, the PF-HI12 at position #4 requires cooling brine, resulting in high cooling costs due to the low temperature of 25.7 °C at the condenser of the second column operated at 131 mbar to enable direct heat
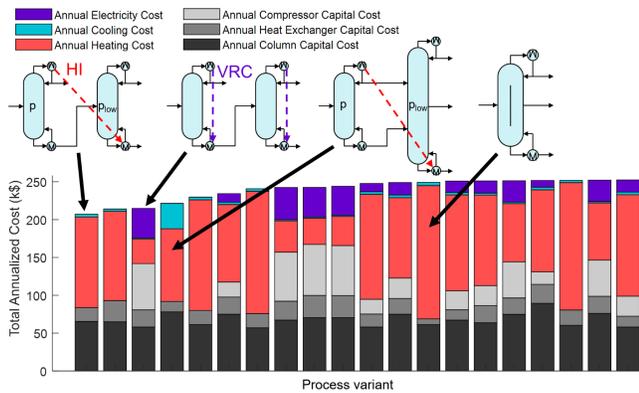
integration.

Figure 3: Distribution of TAC for 20 practically feasible sequences with lowest TAC

To investigate if this configuration yields economic benefits for an increased reference pressure, a sensitivity analysis is performed. As indicated in Figure 4, the PF-HI12 outperforms the DS-HI12 beyond 1.7 bar. From 3 bar on more expensive high temperature steam is required for both sequences. At a reference pressure of 2.25 bar, the PF-HI12 has the lowest TAC (197.7 k$) of all sequences and also ties for the first position regarding net MED (255.2 kW) with a sloppy split with two direct heat integration links.
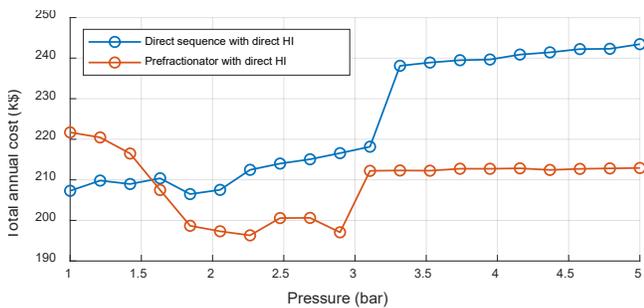

Figure 4: Sensitivity of TAC over pressures for configurations PF-HI12 and DS-HI12

As investment cost and operating costs are competing objectives, the tradeoff is shown in Figure 5 for a reference pressure of 2.25 bar, for all 68 feasible configurations. Here, most VRC variants are excluded due to high discharge temperatures at the increased temperature level. Each of the four non-dominated sequences reflect pareto-optimal solutions. Despite using three columns, a heat integrated sloppy split has the lowest investment costs, closely followed by the DWC, which however requires a difficult-to-control vapor split. The PF-HI12 has the lowest operating costs and lowest overall TAC for the chosen depreciation period and interest rate, but the DS-HI12 is also pareto-optimal, highlighting the value of a multi-objective evaluation.
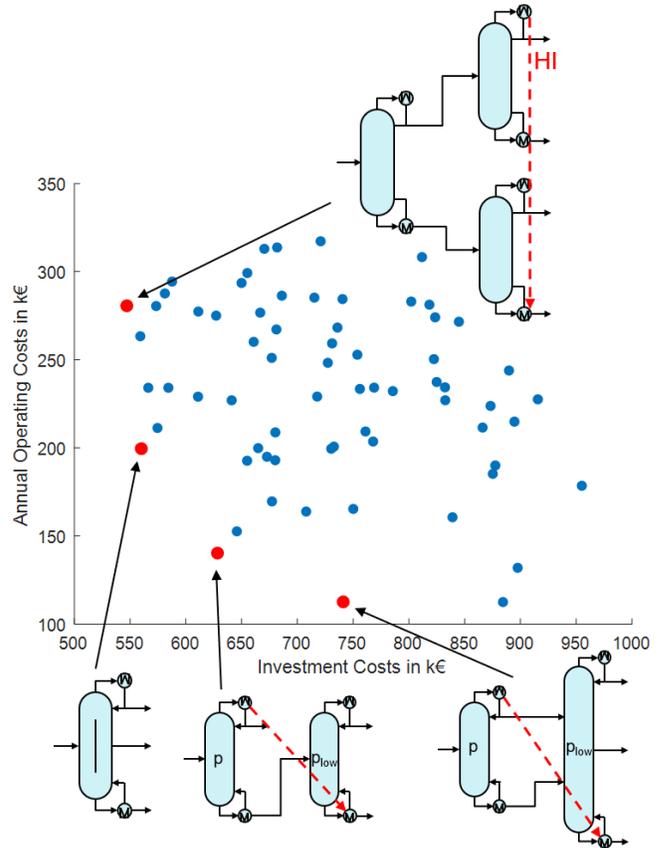

Figure 5: Tradeoff between operating costs and investment costs for 68 practically feasible sequences

4. CONCLUSIONS

An algorithmic framework for the evaluation of more than 750 energy integrated distillation sequences for separation of multicomponent mixtures in three products allows for a quick and quantitative assessment of a range of energy integration methods, covering direct heat integration, thermal coupling, dual- and triple-effect and all possible VRC variants, including combinations with other integration methods. The framework enables a multi-objective evaluation considering the trade-off between energy demand and estimated capital cost, providing interesting insights for a fast identification of most attractive process alternatives under different conditions. The framework will further be extended to cover advanced configurations including liquid only transfer with heat integration [39], and the most promising options will be validated in more detail with MESH-based process optimization [40].

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