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Fast Screening of Energy and Cost Efficient Intensified Distillation Processes

Mirko Skiborowski

Laboratory of Fluid Separations, Department of Biochemical and Chemical Engineering, Technische Universität Dortmund, Emil-Figge-Str. 70, D-44227 Dortmund, Germany
mirko.skiborowski@tu-dortmund.de

While distillation processes still account for the majority of fluid separations, their low thermodynamic efficiency and the resulting high energy requirements raise concerns towards their sustainability in the face of climate change and global warming. Competing technologies, especially various types of membrane processes and hybrid separation processes promise significant improvements in terms of energy efficiency, but are still not applied widely in the chemical industry. So far, the robustness of distillation remains unmatched by these technologies. In order to improve the energy efficiency of distillation processes different means for energy integration have been developed, ranging from the classical direct heat integration, over different forms of thermal coupling, including dividing wall columns, different types of heat pumps, especially mechanical vapour recompression, to multi-effective distillation. In order to evaluate the most energy and cost efficient distillation process all feasible options, or at least a representative number of configurations, should be considered. The most efficient intensified distillation processes is not only the best option based on robust distillation technology, but also the meaningful competitor for all competing technologies. The current contribution presents a screening tool based on accurate shortcut models that account for non-ideal thermodynamics. The screening tool allows for an automatic and computationally efficient evaluation of a large number of alternative intensified distillation processes for the separation of a given mixture into three product streams. It furthermore allows for a scenario-based evaluation of uncertainty information. The applicability is illustrated for several case studies.

1. Introduction

The vast majority of fluid separations in the chemical industry are still performed by means of thermal separations. Especially distillation processes account for about 40% of the total energy consumption in the chemical industry (Sholl and Lively, 2016). Besides alternative separation technologies like membranes, energy integration can facilitate significant improvements of the energy and cost efficiency of thermal separation processes. While a variety of different options for heat integration, thermal coupling and heat pump configurations have been proposed for the reduction of the energy requirements of distillation processes, often only a subset of these options is considered. Especially research articles, which are dedicated to a specific option, often ignore the competing alternatives and advertise large saving potentials on the basis of a comparison with a non-integrated simple sequence of distillation columns. On that basis, e.g. energy reductions of up to 45% for thermal coupling in dividing wall columns (DWC) have been promoted (Kaibel, 2014), while also savings of up to 50% by means of heat pump assisted distillation was promoted (Kiss et al., 2012). While this indicates the possibility of doubling the energy efficiency compared to non-integrated configurations, it also shows that different options provide similar saving potentials. Since the suitability of the available options depends on the specific separation, conceptual design of distillation processes should cover these different options for energy integration in order to determine the most efficient process implementation.
When dealing with the problem of separating a given multicomponent mixture into several products, there are usually multiple process configurations possible. In case of zeotropic mixtures, the number of possible simple sequences of sharp splits and thermally coupled configurations, especially DWC, can be determined a-priori (Thompson and King, 1972; Zhang et al., 2017). More importantly, all these sequences as well as the options

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for thermal coupling can be generated automatically (Agrawal, 2003; Shah and Agrawal, 2010). An elaborate description of the conceptual design of zeotropic distillation processes, including simple sequences and thermal coupling, can be found in the book chapter of Shah and Agrawal (2014).
However, only few design methods consider the evaluation of competing alternatives for energy integration, beyond simple sequences and thermal coupling. In their recent publication, Cui et al. (2016) mandate the necessity of such an assessment and the availability of a tool for quick decision making. They furthermore present a shortcut method to choose between mechanical vapour recompression (MVR) and multi-effect distillation (MED) for the separation of binary systems. Based on an elaborate literature study, Kiss et al. (2012) present a selection scheme of energy efficient distillation technologies, with a special focus on heat pumps. For the separation of multicomponent mixtures, of course different sequences have to be considered and for each sequence the different means for energy integration should be assessed. Direct heat integration and multi-effective distillation usually require the modification of the operating conditions, specifically the operating pressure. Thereby, the temperature levels in the reboiler and condenser can be shifted such that the level of integration can be maximized. Nevertheless, this combination of work and heat integration results in a more complex problem (Fu et al., 2017).
In order to provide accurate estimates of the energy requirement for the separation of non-ideal mixtures, it is also of specific importance to avoid simplifying assumptions like constant relative volatilities (CRV) and constant molar overflow (CMO). Yet, most design methods rely on such assumptions, applying e.g. the Underwood model for the evaluation of minimum energy duties. While a number of thermodynamically sound shortcut methods is available (Skiborowski et al., 2014), only the approach of Brüggemann and Marquardt (2005), which is again limited to simple sequences and thermal coupling, makes use of such a method.
In order to overcome the reported limitations, the current article proposes a systematic screening procedure by means of a full enumeration of a large number of process variants based on a reliable shortcut method. Overall more than 30 process configurations, including heat-integration between single columns, thermal coupling by means of side stripper/rectifier configurations and DWCs, MED and the application of MVR, based on isentropic compression, are considered for the separation of a multicomponent mixture into three product streams. Each of these configurations can be automatically evaluated for several hundred different scenarios within just a few minutes. Thereby, the uncertainty associated to feed and product specifications, utility costs and the thermodynamic model can be efficiently evaluated.

2. Method

In order to evaluate the alternative process configurations automatically an algorithmic framework was developed, which is illustrated in Figure 1. The evaluation of the minimum energy requirement of each individual distillation column builds on the thermodynamically sound pinch-based rectification body method (RBM) (Bausa et al., 1996). The RBM assumes an infinite number of equilibrium stages in order to determine the minimum energy requirement. Since it does not rely on CMO and CRV assumptions, it is applicable to non-ideal and azeotropic mixtures. The computationally efficient implementation in C includes different thermodynamic models and allows for the application to different mixtures by merely providing a property data file with appropriate property parameters.

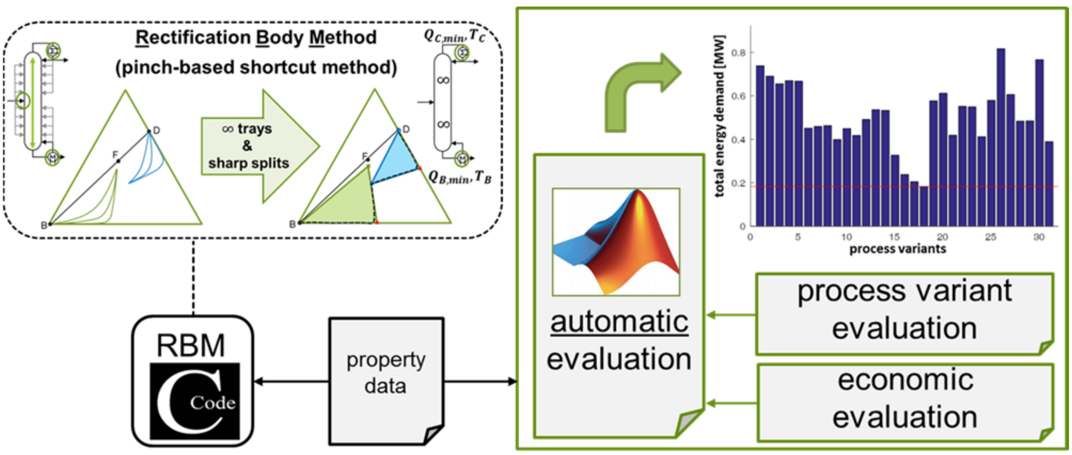

Figure 1: Algorithmic framework for the fast screening of various intensified distillation processes

All of the process variants, which will be introduced more closely in the following subsections, are evaluated in a Matlab toolbox that determines the minimum energy requirement of each variant based on dedicated programs. The specific programs also perform an optimization of the operating points, in case this is required. Furthermore, a subsequent evaluation of the operating costs, based on the energy requirements and the required utilities, are performed in order to identify the economically favorable option.

2.1 Simple column configurations

A multicomponent mixture can generally be separated into three product streams by means of the well known direct split (DS), the indirect split (IS) and the intermediate split (MS) sequence. While the first two variants require just two columns, the latter requires three columns. The minimum energy requirement of the intermediate split sequence is obtained for an optimal distribution of the intermediate product in the first column, which results in the so-called preferred split. This distribution is determined by an optimization of the split factor of the intermediate product (ϕ_B) , in accordance with the illustration given in Figure 2.

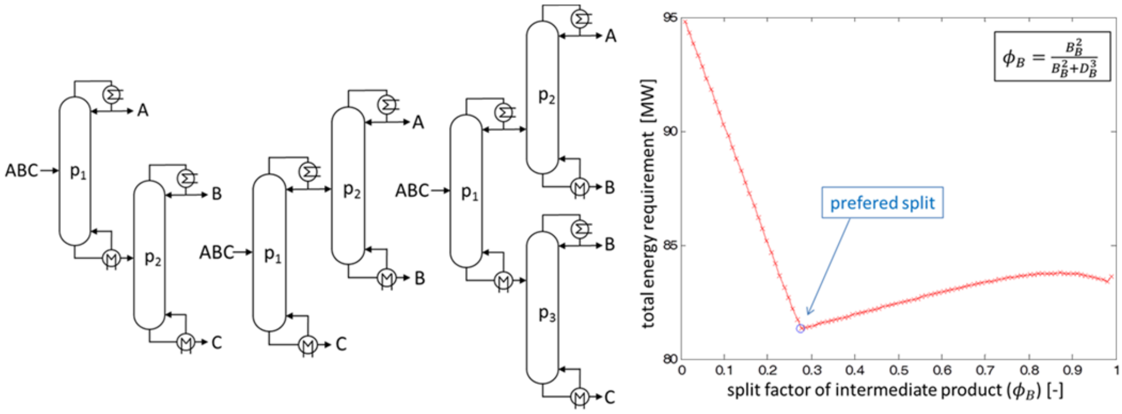

Figure 2: Illustration of direct, indirect and intermediate split (left side), as well as the energy requirements of the intermediate split for a variation of the split factor of the intermediate product ϕ_B (right side).

2.2 Thermally coupled configurations

In accordance with the simple sequences, six thermally coupled configurations are derived and evaluated. Based on the decomposition approach proposed by Carlberg and Westerberg (1989) a side rectifier, a side stripper and different pre-fractionator configurations are evaluated. The side rectifier and the side stripper configuration can be implemented as DWC with a dividing wall at the top, or at the bottom. Furthermore, two configurations with partially coupled pre-fractionator (condenser or reboiler) and a fully coupled pre-fractionator configuration are evaluated. The latter corresponds to the so-called Petlyuk configuration, which can be implemented in form of a DWC with a dividing wall in the center. This is illustrated in Figure 3.

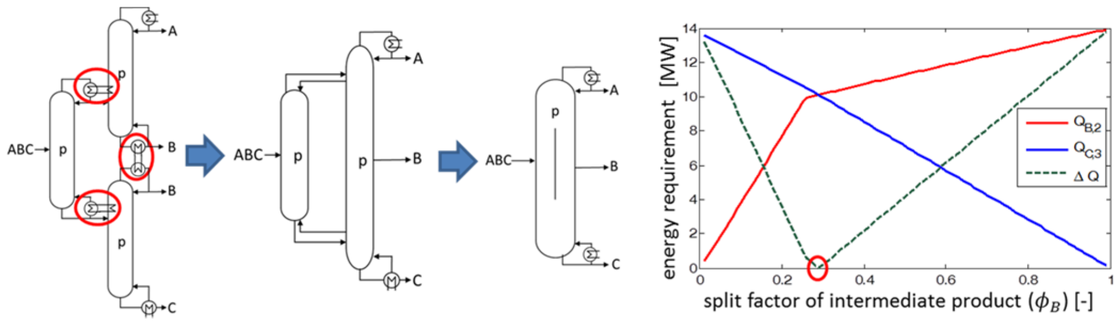

Figure 3: Illustration of the transformation of the intermediate split sequence to the DWC (left side) and the required split factor of the intermediate product $\phi_B$for an equilibration of the heat duties of $Q_{B,2}$ and $Q_{C,3}$.

In order to achieve the concurrent inter-column heat coupling between the reboiler of the upper subsequent column ($Q_{B,2}$) and the condenser of the lower subsequent column ($Q_{C,3}$), a minimization of their absolute difference (ΔQ) is performed, similar to the work of Brüggemann and Marquardt (2005). For further elaborate description of the decomposition and reformulation approaches for the thermally coupled processes refer to the work of Brüggemann and Marquardt (2005) and the recent review of Waltermann and Skiborowski (2017).

2.3 Direct heat integration

Overall six different options for direct heat integration are evaluated for the simple sequences. For each of these options the operating pressure of at least one column is modified to facilitate a minimum temperature difference of 10K between the streams considered for heat integration. The necessary operating pressure is determined by a series of flash calculations while the enthalpy difference between the saturated liquid states of the feed stream at the different pressure levels is considered as additional heat requirement. Table 1 lists the heat duties of the integrated heat exchangers for the different sequences, as well as the variable pressure, which is adjusted to warrant the necessary minimum temperature difference. In case the heat duties do not match, the remaining heat requirement is satisfied by an external heat source, taking into account the appropriate utility in the final economic evaluation

Table 1: List of the heat duties of reboiler (Q_B) and condenser (Q_C) of specific columns considered for heat integration for the different simple column configurations, as well as the modified variable pressure.

configuration	DS	IS	MS_1	MS_2	MS_3	MS_4
Integration between	$Q_{B1} \leftrightarrow Q_{C,2}$	$Q_{B2} \leftrightarrow Q_{C,1}$	$Q_{B2} \leftrightarrow Q_{C,1}$	$Q_{B1} \leftrightarrow Q_{C,3}$	$Q_{B2} \leftrightarrow Q_{C,3}$	$Q_{B2} \leftrightarrow Q_{C,1}$ & $Q_{B1} \leftrightarrow Q_{C,3}$
variable pressure	p_2	p_1	p_1	p_3	p_3	p_1 & p_3

2.4 Mechanical vapor recompression

Heat pumps allow for a direct heat integration between the condenser and reboiler of a single column. While different types of heat pumps can be applied, mechanical vapor recompression is the state-of-the-art solution. It saves not only one of the heat exchangers, but also comes close to the potential energy savings that can be achieved by so-called heat-integrated distillation columns (HiDiCs) (Harwardt and Marquardt, 2012). However, the required compressor constitutes a significant investment and requires electrical energy. In order to account for the necessary investment in the economic evaluation, its depreciation is considered as part of the operating costs, while the electrical energy is considered with a factor of two in the evaluation of the total energy demand. The minimum pressure stroke for compression is again determined by a series of flash calculations and the minimum workload for compression is determined based on an isentropic compression with an isentropic efficiency of 80% and mechanical efficiency of 90%. Additional heat loads for supersaturation prior to the compressor and the compensation for remaining heat requirements are accounted for in the evaluation of the process.

2.5 Multi effect distillation

Similar to MVR, heat integration in MED can be performed for each split individually. Therefore, the feed stream is split into two fractions, which are processed at different pressure in separate columns, such that the condensation of the top vapor stream of the high pressure column provides the energy required for the reboiler of the low pressure column. The determination of the optimal pressure level is performed similar to the direct heat integration options. Overall, thirteen MED variants are evaluated for the three simple column configurations, by considering MED for each individual column as well as the combination of columns.

3. Case studies

In order to demonstrate the applicability and computational efficiency of the developed algorithmic framework two case studies for the separation of a ternary zeotropic mixture and a quaternary azeotropic mixture are presented. Furthermore a multi-scenario evaluation is presented for the separation of the ternary mixture, which allows for the evaluation of the impact of uncertainty information on the obtained results. All computations have been performed on an Intel Core™ i5-6440HQ CPU with 2.6Ghz using Matlab R2016a.

3.1 Separation of a ternary mixture of benzene, toluene and ethylbenzene

As the first case study, a saturated feed stream of 10 mol/sec of the ternary mixture of 70 mol% benzene, 20 mol%, toluene and 10 mol% ethylbenzene is to be separated into approximately pure products. The thermodynamic properties are determined based on the Wilson model, the extended Antoine equation, as well as DIPPR correlations for the specific heat capacities and heat of vaporization. The results of the evaluation of the 31 process variants considered in the current implementation of the algorithmic framework are illustrated in Figure 4. The complete evaluation of all process variants and the economic assessment require less than 30 CPU sec. The MVR for the direct split sequence allows for the highest energy reduction. Even compared to the best option without the use of a compressor, the MED variant for both columns in the same sequence, the MVR variant still saves 35% of the energy requirement.

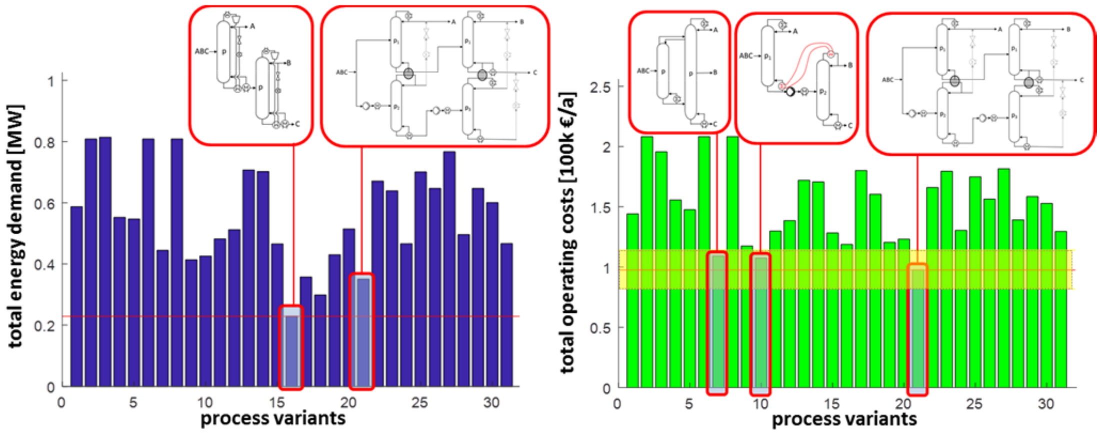

Figure 4: Illustration of the resulting total energy requirements (left) and total operating costs (right), for the separation of the ternary benzene, toluene, ethylbenzene mixture.

However, due to the significant costs of the compressor, the MVR variant is less attractive in terms of the operating costs, for which the MED process becomes the most favourable solution. In comparison with the direct split without heat integration, the MED variant results in energy savings of 40% and an operating cost reduction of 32%. However, other options for energy integration are competitive to the MED variant. The pre-fractionator with a partially coupled condenser and the direct heat integration for the direct split require only a 10% increase in the operating costs and are comparably simpler process options, which presumably require a much smaller investment. Therefore, they should subsequently be investigated in terms of a detailed design.
This result is further fostered by an investigation of the sensitivity of the results on uncertainties in the process specifications, the thermodynamic model and the economic parameters. These uncertainties are evaluated by means of a multi-scenario evaluation, for which the composition of the feed stream is slightly varied by ±2mol% for benzene and ethylbenzene, the alternative use of the Uniquac model, as well as modifications of ±15% for the utility costs. Considering all possible variations, taking into account the lower bound, mean value and upper bound for each parameter, 1458 scenarios are evaluated. The results, which are obtained in less than 5 min of CPU time, indicate cost variations of ±17% for the most attractive MED option (indicated by the yellow beam in Figure 3).

3.2 Separation of a quaternary mixture of acetone, chloroform, benzene and toluene

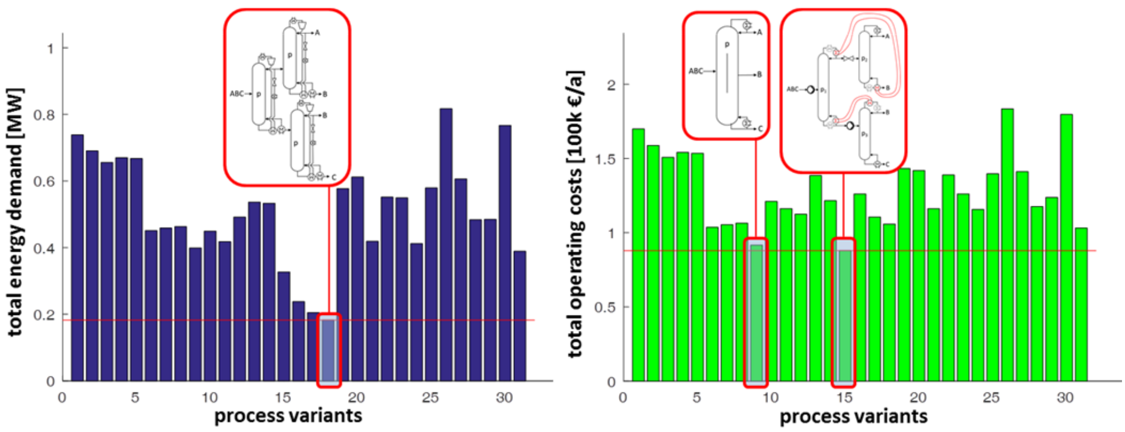

Figure 5: Illustration of the resulting total energy requirements (left) and total operating costs (right), for the separation of the quaternary acetone, benzene, chloroform, toluene mixture.

In the second case study, a saturated feed stream of 10 mol/sec of the quaternary mixture of 4 mol% acetone, 10 mol% chloroform, 43 mol% of benzene and 43 mol% of toluene is to be separated in a product stream containing all the acetone and chloroform and two approximately pure product streams of benzene and toluene. This separation is feasible by means of distillation, although the mixture exhibits a binary azeotrope between acetone and chloroform and an according distillation boundary. The thermodynamic properties are determined based on the Wilson model, the extended Antoine equation, as well as a polynomial correlation for the specific heat capacities and the Watson model for the heat of vaporization. The results of the evaluation are illustrated in Figure 5. Similar to the previous case study, the MVR variants allow for the separation with the lowest energy requirements, yet again not providing the most economical option. While a DWC equivalent to the Petyluk configuration is very attractive from the economic point of view, the intermediate split with direct heat integration between all three columns (configuration MS_4 in Table 1) is the most promising configuration in terms of the total operating costs. Both options save about 40% of the operating costs compared to the best simple column configuration. The direct heat integrated variant requires even 20% less energy, but requires a more expensive utility for the reboiler of the third column, which is operated at elevated pressure. Since this configuration requires three individual columns it is also presumably less attractive than the DWC in terms of economics, when investment costs are considered as well.

4. Conclusion

The current article proposes an extensive algorithmic framework for the evaluation of the most promising distillation configurations, considering a variety of options for energy integration. The evaluation is not based on limiting assumptions like CMO or CRV, such that it can be applied to the separation of non-ideal multicomponent mixtures. The case studies demonstrate the computational efficiency of the current approach and highlight the usefulness in identifying the true potential of different process configurations by means of an elaborate comparison with alternative options. Usually different options allow for significant energy savings compared to the non-integrated process variants. Since equipment sizing and capital cost estimation is not part of the shortcut screening, the most promising options should further be investigated by means of a more detailed process optimization, as proposed by Waltermann and Skiborowski (2016).

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