

Can Simple Side Stream Configurations Compete with Fully Thermally Coupled Dividing Wall Columns?

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Abstract. It is well known that thermal coupling of distillation columns can substantially decrease the energy requirements of distillation processes, which is confirmed by several hundred industrial implementations of dividing wall columns. However, the respective vapor splits have to be properly designed and require consistent hydrodynamics in the adjacent column sections. These limitations can be overcome by transformation of the thermal coupling to a side stream configuration, which adds a degree of freedom for operation of the process and allows the columns to be operated at different pressures. The current study investigates energy requirements and operating costs of single side stream configurations thermodynamically equivalent to side-rectifier and side-stripper columns in comparison to fully-thermally coupled dividing wall columns and heat-integrated configurations. While side-stream configurations provide an interesting retrofit option and are competitive to fully-coupled dividing wall columns for certain ranges of feed compositions, they can outperform them significantly exploiting additional heat integration.

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1. Introduction

In order to mitigate the consequences of climate change, there is a great need to reduce the energy demand and greenhouse gas emissions in the chemical industry, which ranges among the largest consumers of energy worldwide. The majority of energy is used for thermal separations, with distillation processes as the most dominant technology and the largest share of the respective energy consumption (Sholl and Lively, 2016). Besides the combination of distillation with other separation technologies such as extraction or membrane separations to hybrid separation processes, different direct options for improving the energy efficiency in distillation processes have been established (Blažušiak et al., 2018). Direct heat integration, multi-effect distillation, dividing wall columns (DWCs), as well as mechanical vapor recompression and internally heat-integrated columns, so called HIDiC, allow for energy savings of up to 50 % (Kiss, 2014).

The thermal coupling of distillation columns, which replaces individual heat exchangers by a bi-directional vapor and liquid transfer, as well as the equipment integrated implementation as a DWC are well-established options with several hundred industrial implementations (Lukač et al., 2019). These configurations enable energy and operating cost reductions of 30-40 % compared to non-integrated process configurations and up to 30 % reduced investments for DWCs (Waltermann et al., 2019).

However, these benefits come with certain challenges both in process design and operation. The optimal design of DWCs is considerably more complex than the design of column sequences and the operation and control of thermally coupled columns is significantly more challenging due to the nonlinear nature of the process (Weinfeld et al., 2018). While it has been shown that DWCs can be controlled effectively (Rewagad and Kiss, 2012), the vapor split is usually not part of the control structure (Staak et al., 2014) and the pressure profiles in the adjacent column sections adjust themselves based on the pressure drop during operation. This requires an optimal placement of the dividing wall during process design and prohibits the possibility of further heat integration, resulting in a loss of design flexibility.

In order to overcome the latter limitations, thermally coupled configurations can generally be modified by adding column sections and heat exchangers in such a way, that the bi-directional vapor and liquid exchange is replaced with a liquid only transfer (LOT) stream (Agrawal, 2000). While the equipment costs increase, the energy saving potential of the thermally coupled configuration is retained because the resulting LOT configuration is thermodynamically equivalent (Ramapriya et al., 2016). The LOT configuration further allows for a hydrodynamically independent

operation of the individual columns, providing further potential for heat integration as recently shown for an LOT side rectifier with additional heat integration (Skiborowski, 2020).

The current work extends the previous investigations for LOT side rectifier and side stripper configurations, which both represent potential retrofit options for existing direct and indirect column sequences by implementation of a single side stream. The energy and cost saving potential of these LOT configurations is first introduced through a systematic transformation of the side stripper and side rectifier and furthermore analyzed without and with additional heat integration in comparison with fully coupled DWCs and heat-integrated column sequences by means of a shortcut-based framework. The performance is evaluated with respect to the minimum energy requirements and operating costs for the separation of a benzene, toluene and ethylbenzene mixture, as well as a mixture of hexanol, octanol and decanol.

2. Methods

Section 2.1 and 2.2 introduce the LOT side stripper and rectifier configurations without and with heat integration. Subsequently, section 2.3 and 2.4 outline the applied approach for computation of the minimum energy demand (MED) of the novel configurations and the screening of the competing configurations for the respective chemical systems.

2.1. LOT side stripper with potential heat integration

The thermally coupled side stripper can be converted to a thermodynamically equivalent LOT configuration in three consecutive steps (Agrawal, 2000). In the first step shown in Fig. 1, the rectifying section and condenser of the main column are copied and positioned above the side column. Next, the vapor transfer stream is redirected to the copied top section, which is finally joined with the side column. In the resulting LOT side stripper configuration, both columns are connected via a single liquid side stream from the first column to the second column.

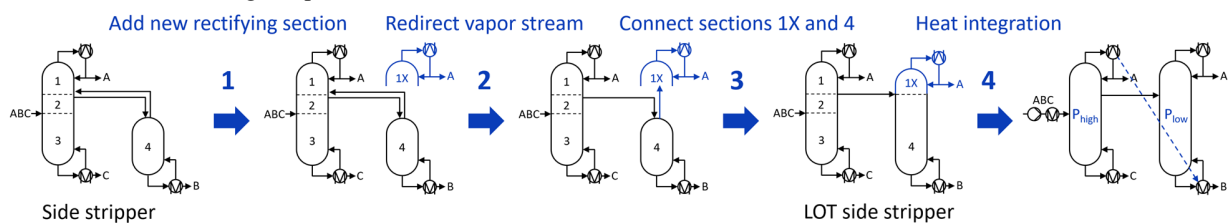


Fig. 1 Three step transformation from a conventional side stripper configuration to a LOT side stripper and fourth step for heat integration

While the energy demand of the LOT configuration is equivalent to that of the side stripper, the LOT configuration enables operation of both columns at individual pressure, which can further be exploited for additional heat integration if the boiling point of the top product in the first column is raised above the boiling point of the bottom product in the second column. This is either accomplished by increasing the operating pressure of the first column or by decreasing the operating pressure of the second column. In the current study, only the pressure in the first column is changed, which provides a more conservative estimate of the potential performance. The pressure is increased by a pump in the feed stream and an additional heat exchanger is introduced to maintain a liquid boiling feed.

2.2. LOT side rectifier with potential heat integration

The side rectifier configuration can be converted into a side rectifier with LOT with similar transformation steps as shown in Fig. 2. First, the bottom section of the main column including the reboiler is copied and placed below the side column. Next, the vapor transfer stream is eliminated and substituted by vapor from the copied bottom section. Finally, the side column and the new bottom section are joined.

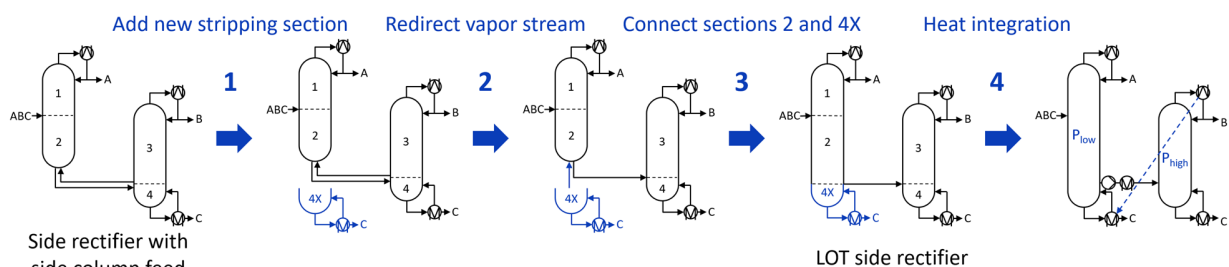


Fig. 2 Three step transformation from a conventional side rectifier configuration with side column feed to a LOT side rectifier and fourth step for heat integration

In the case of a heat-integrated LOT side rectifier, either the pressure of the second column is increased, or the pressure of the first column is reduced, in order to raise the temperature of the top product of the second column above the boiling temperature of the bottom product of the first column. In the current study, only the pressure in the second column is changed and increased by a pump in the side stream, which again provides a conservative estimate of the performance of this configuration. An additional heat exchanger is introduced to maintain a liquid boiling feed.

2.3. Minimum energy demand computation of LOT configurations

The performance of the LOT configurations without and with heat integration is analyzed based on the MED and the respective operating costs, accounting for the different utilities required for cooling and heating. For that purpose, the MED of the individual columns is determined by means of the Rectification Body Method (RBM), which is a pinch-based shortcut method that does not require constant relative volatility and constant molar overflow assumptions (Bausa et al., 1998). Since the LOT configurations are thermodynamically equivalent to the basic side stripper and side rectifier configurations, the MED of these configurations can be estimated based on the decomposition approach of Carlberg and Westerberg (1989), as illustrated for the RBM by von Watzdorf et al. (1999). However, in order to evaluate the possible heat integration, it is important to know the amount and composition of the side stream and the individual heat duties of both columns. Therefore, the MED of the LOT configuration is determined based on the MED of the individual columns, determining the optimal amount of the low (high) boiling product in the side stream for the side stripper (rectifier) by means of a simple bisection.

For the LOT configurations with additional heat integration, the necessary operating pressure of the heat supplying column is first determined by means of flash calculations, such that the boiling temperature of the top product is 10 K above the boiling temperature of the bottom product of the connected column. Subsequently, the MED of the heat-integrated configuration is determined by means of a similar bisection approach, considering the distribution of the low (heavy) boiling product, while simultaneously accounting for the heat duty required to preheat the feed of the heat supplying column as well as any additional heating or cooling duty required to compensate for a mismatch between the condenser and reboiler duty of the heat-integrated columns.

2.4. Screening for energy demand and operating costs

In order to evaluate the presented LOT configurations without and with heat integration, their performance needs to be compared with alternative column configurations. While the improvement potential of intensified distillation processes is frequently reported with respect to the non-integrated sequences, it is of special interest to analyze the performance regarding alternative intensified options. In this case, the most interesting alternatives are the individual thermally coupled configurations and the heat-integrated column sequences in order to determine if and under which conditions the combined heat-integrated LOT configurations are beneficial. Overall, the MED estimates are evaluated for a total number of 14 process configurations.

For this comparison, the newly developed LOT side stripper and side rectifier configuration without and with heat integration are implemented in a previously presented shortcut-based screening tool (Skiborowski, 2018). In order to analyze the potential performance on a broader basis, the individual process MEDs and operating costs are determined for varying feed compositions which cover the whole range of potential feed compositions by 171 equally distributed samples. This results in the evaluation of the MED for 2394 feed and process combinations and additional operating cost estimates for the separation of one chemical system.

3. Case Studies

The separation of two zeotropic mixtures is investigated. The first system of benzene, toluene and ethylbenzene is evaluated with a base pressure of 1.013 bar and VLE computations based on the Wilson model. The second mixture of higher boiling alcohols hexanol, octanol and decanol is evaluated at a base pressure of 0.08 bar and VLE computations based on the UNIQUAC model. The heat of vaporization and specific heat capacities are calculated with DIPPR correlations. All property parameters are imported from Aspen Plus. For both systems, the available utilities are cooling water at 27 °C and a cost of 0.6 \$/GJ, medium pressure steam at 10.3 barg (185.5 °C) and 4 \$/GJ and high-pressure steam at 41.7 barg (253.8 °C) and 6 \$/GJ.

3.1. Energy and operating cost screening without heat integration

In order to evaluate the question raised in the title of this contribution, the LOT configurations are first evaluated in comparison to the simple sequences and the DWC. As to be expected, the fully-coupled DWC is the most favorable configuration regarding MED as well as operating costs for all feed compositions of both substance systems. While thermodynamically equivalent LOT configurations to a DWC can be designed, these require a second side stream and

complicate further heat integration, as both columns produce the low and high boiling product as top and bottoms stream (Ramapriya et al., 2016). Consequently, it is of interest to analyze under which conditions the LOT configurations without heat integration perform only slightly worse than the fully-coupled DWC. For this purpose, Fig. 3 illustrates the second most favorable configuration in terms of MED and annual operating costs for the separation of the benzene, toluene, ethylbenzene mixture. The results are qualitatively very similar for the alcohol system, which are therefore not further discussed. The symbols in the diagram indicate which configuration is the second best with respect to the specific feed composition.

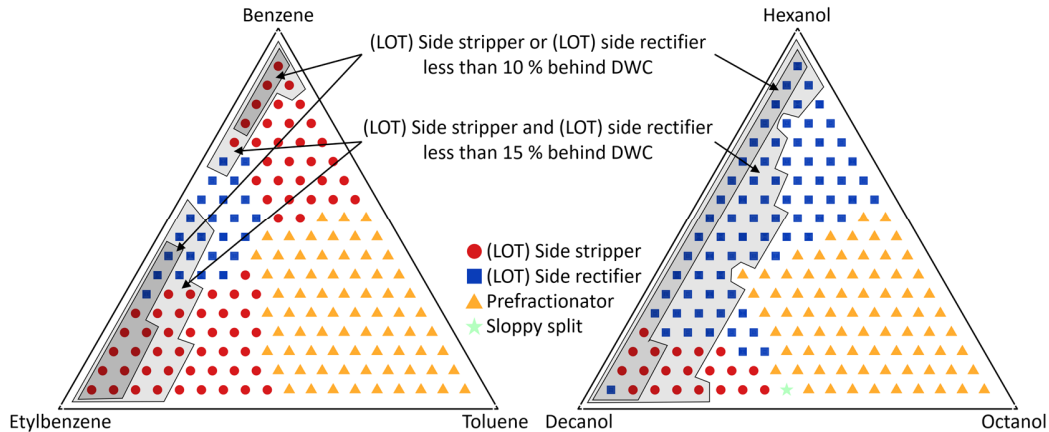


Fig. 3 Second most favorable configuration without heat integration regarding minimum energy demand and costs for different feed compositions of benzene, toluene and ethylbenzene (left) and hexanol, octanol and decanol (right)

The side stripper and side rectifier and the thermodynamically equivalent LOT configurations are the second-best option for more than half of the feed compositions. Especially at high concentrations of the light boiling product and the heavy boiling product, these configurations come close to the fully thermally coupled DWC with a margin of less than 10 % in terms of MED and operating costs. In these cases, a retrofit of an existing simple sequence by means of a single side stream may be of special interest. Only in case of large fractions of the intermediate boiling product, both configurations are outperformed by the prefractionator configuration as second-best option.

3.2. Energy and operating cost screening with heat integration

In order to evaluate the potential of the LOT configurations with heat integration, the screening is extended to include all heat-integrated sequences. Fig. 4 presents the best configuration with respect to MED (left) and annual operating costs (right) for the separation of the benzene, toluene and ethylbenzene mixture. Including heat integration, the fully thermally coupled DWC is only favorable for ~ 12 % of feed compositions, while heat-integrated direct splits and sloppy splits require the lowest MED and operating costs for feed compositions with high amounts of intermediate boiling products.

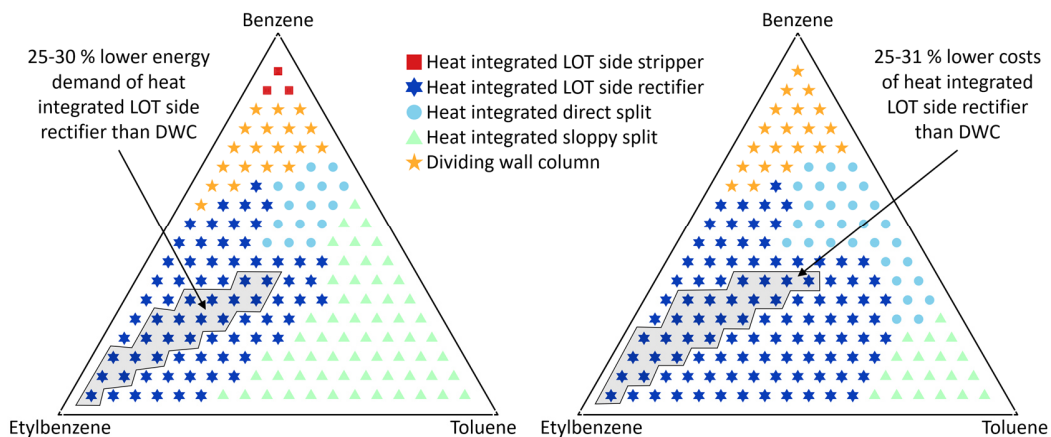


Fig. 4 Best configurations regarding energy (left) and costs (right) for different feed compositions of benzene, toluene and ethylbenzene

The heat-integrated LOT side stripper offers the lowest MED for feed compositions with very high benzene content. However, these MED benefits do not transfer to operating costs for the considered utilities, since high pressure steam is required for the high-pressure column. Consequently, the DWC has lower operating costs for these few feed compositions. The heat-integrated LOT side rectifier offers the lowest MED and operating costs for a wide range of feed compositions (> 40 %). Moreover, both MED and operating costs of this configuration are over 25 % lower compared to the fully thermally coupled DWC for ~ 12 % of feed compositions with a high content of high boiling product and almost equivalent shares of low and heavy boiling product. In the best case, the MED and operating costs of the heat-integrated LOT side rectifier are about 30 % lower compared to the fully thermally coupled DWC and about 27 % lower than a heat-integrated direct split, which in this case are the third- and second-best options.

The results of the MED-based screening are very similar for the separation of the hexanol, octanol and decanol mixture. Fig. 5 illustrates the best performing configurations regarding MED (left) and annual operating costs (right). The most noticeable differences with respect to the MED are a shift in the range of compositions for which the DWC provides the lowest MED and a larger share of compositions for which the heat-integrated direct split outperforms the heat-integrated sloppy split. While the heat-integrated LOT side stripper is not recognized as a superior option in the sample set, the heat-integrated LOT side rectifier is again identified as most favorable option in terms of MED for ~ 40 % of the feed compositions and can save up to 16.5 % of energy compared to the next best alternative and up to 24.9 % in the shaded region relative to a fully thermally coupled DWC. These savings do however not transfer to the operating costs for the considered utilities and the DWC is determined as best option for about half of the feed compositions in terms of costs.

This difference can be explained by the different boiling temperature of the bottom products of these configurations. In order to perform a direct heat integration for the LOT side rectifier, the pressure in the second column is raised to 0.3728 bar. This results in an increase of the boiling temperature of the heavy product decanol from 151.7 °C at 0.08 bar to 194.2 °C, mandating the more expensive high-pressure steam, whereas medium-pressure steam is sufficient for the DWC. Obviously, these results depend strongly on the availability and cost of the respective utilities. Furthermore, the current evaluation focuses on the conservative approach of operating the high-pressure column at increased pressure as previously described. Alternatively, the low-pressure column could be operated at decreased pressure to avoid the use of high-pressure steam, thus conserving the MED benefits for the operating costs if the condenser can still be operated with cooling water. For the overall results it is also important to note that the heat-integrated sloppy split configuration, which is determined as favorable for a wide range of feed compositions, requires three individual columns. Therefore, it comes with a considerable increase in investment costs, which is not evaluated in the current shortcut screening.

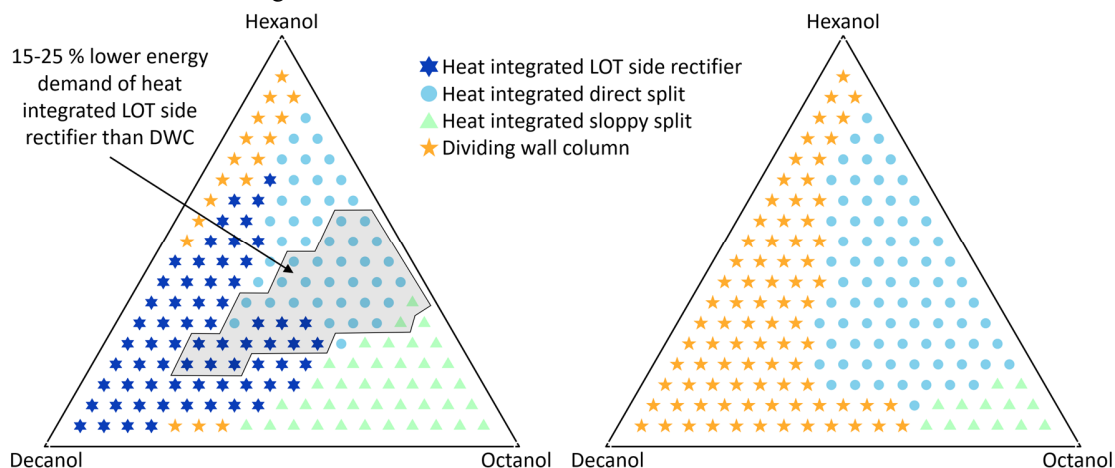


Fig. 5 Best configurations regarding energy (left) and costs (right) for different feed compositions of hexanol, octanol and decanol

4. Conclusion

The vapor streams between columns of a thermally coupled configuration can be eliminated by the concept of liquid only transfer, which enables a more flexible operation and a potentially simple retrofit of existing columns, while retaining the energy-saving potential of the thermal coupling. When considering a single side stream configuration, the same energy savings obtained by a side rectifier and side stripper can be reached. These come fairly close (less

than 10 % higher) to the saving potential of the fully thermally coupled dividing wall column for a wide range of feed compositions with low amount of the intermediate boiling product. While not explicitly addressed in the current study, a configuration with two LOT side streams allows for the same energy savings as offered by a fully thermally coupled dividing wall column.

Despite the lower potential for energy savings by the partial thermal coupling, the LOT side rectifier and side stripper configurations offer additional advantages, since both columns can be operated at individual pressure. Thus, they may not only be applied in cases in which individual pressures are required, but also exploit a potential combination of (partial) thermal coupling and heat integration. As illustrated for the two evaluated case studies, heat-integrated LOT side stripper and especially side rectifier configurations provide the lowest energy demand for a wide range of feed compositions and can save up to 30 % of the energy requirement of the fully thermally coupled dividing wall column, which depending on the available utilities and their costs may directly translate into respective operating cost savings.

Consequently, it can be concluded that depending on the specific separation task, simple side stream configurations, which implement the LOT equivalent of a side stripper or side rectifier, can closely approach the energy requirements of a fully thermally coupled dividing wall column and may significantly reduce these energy requirements in the case of additional heat integration. Depending on the available utilities, these savings can directly be transferred to operating cost savings. However, the additional pressure modification may also require more expensive utilities and thereby consume the potential energy savings. Consequently, a case specific evaluation is important in order to identify the optimal choice for a specific application, for which the shortcut screening tool provides an excellent basis. Despite the possibly large energy savings, the LOT side rectifier and stripper do of course maintain the limitation of thermal coupling that heat transfer is required at more extreme temperature levels, which is further extended by the additional heat integration. While this may or may not be reflected by the utilities, it is generally reflected by consideration of the exergy loss and further investigations will also consider the thermodynamic efficiency.

Acknowledgements

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