Energy Efficient Distillation by Combination of Thermal Coupling and Heat Integration

Mirko Skiborowski

TU Dortmund University, Department of Biochemical and Chemical Engineering, Laboratory of Fluid Separations, Emil-Figge-Strasse 70, 44227 Dortmund, Germany
mirko.skiborowski@tu-dortmund.de

Abstract
Conventional heat-integration between adjacent columns, as well as thermal coupling and the equipment-integrated implementation in a dividing wall column are successful concepts for the improvement of the energy efficiency of distillation processes. While especially dividing wall columns have made a considerable impact in industrial application, further heat integration is prevented by the bidirectional transfer of liquid and vapor streams that impede a necessary pressure variation for modification of the boiling temperatures. This limitation can however be overcome by the modification of thermal couplings to one-directed liquid only transfer. While this concept has been proposed almost 20 years ago, it has received limited attention so far. In order to evaluate the prospect of this combination, the current article exploits a combination of a shortcut-based screening and a rigorous economic optimization, in order to evaluate a heat-integrated side-rectifier with liquid only transfer modification in comparison with a range of alternative options. The application to an exemplary case study highlights the huge potential of this combination, showcasing the possibility to save half of the energy required for a non-integrated configuration and even more than 30% compared to fully thermally coupled configurations, depending on the feed composition.

Keywords: distillation, thermal coupling, heat integration, rectification body method

1. Introduction
Despite serious concerns about the low thermodynamic efficiency, distillation processes remain the working horse for fluid separations, especially in case of large scale continuous production processes. Besides the exploitation of hybrid separation processes, combining distillation with other technologies such as extraction and membrane separations, a number of options for improving the energy efficiency in distillation processes have been established. These include e.g. direct heat integration and multi effect distillation, thermal coupling and the equipment integrated dividing wall columns (DWC), mechanical vapor recompression (MVR) and internally heat integrated columns, so called HiDiC (Kiss et al., 2012). The individual concepts allow for energy savings of up to 50% compared to the non-integrated distillation processes. Yet, choosing the right option requires a case specific evaluation of the different process concepts, which can be performed by means of shortcut methods (Skiborowski, 2018), as well as rigorous economic optimization of MESH based superstructure models (Waltermann and Skiborowski, 2019). While some combinations of these concepts have recently been considered in case-specific evaluations, such as the combination of MVR and DWC (Jana, 2019; Patraşcu et al., 2018) or the extension of a HiDiC with further MVR through intermediate heat
exchangers (Kiran and Jana, 2016), such evaluations are still scarce. An interesting combination of thermal coupling and heat integration has been proposed by Agrawal (2000a) almost two decades ago. However, despite the indicated prospect of these so-called double-effect thermally coupled configurations, which were evaluated based on very approximate calculation for theoretical mixtures with constant relative volatility, the concept has received little attention so far. While thermal coupling itself and DWC in specific are considered as one of the most prominent examples of process intensification in fluid separations, with more than 130 industrial-scale DWC implementations (Staak et al., 2014), a direct extension of these configurations to the aforementioned combination is infeasible, due the standard bidirectional transfer of liquid and vapor streams between thermally coupled column sections that impedes the necessary pressure variation. This variation only becomes feasible in case of a transformation of the thermal coupling to a one-directed liquid only transfer (LOT), as introduced by Agrawal (2000b) and more recently considered in a systematic generation of DWC configurations with LOT modifications that allow for an independent control of the vapor flow rate in each partitioned zone of the DWC (Madenoor Ramapriya et al., 2014). Apart from the improved operability, Jiang and Agrawal (2019) conclude that the possibility to combine heat-integration with thermal couplings is another major opportunity offered by the LOT modification, since even double-effect systems for basic configurations can oftentimes outperform the best DWC configurations.

In order to evaluate this potential, the current study performs an optimization-based evaluation of a heat-integrated side-rectifier with LOT modification with various competing process concepts. The evaluation is based on a combination of pinch-based shortcut models, as well as rigorous equilibrium-stage models for an economic process optimization. The results obtained for a representative case study on the separation of a benzene, toluene, ethylbenzene mixture illustrates the significant potential for process intensification by showcasing energy savings of more than 30% in comparison to the fully thermally coupled DWC and the superiority for a wide range of feed compositions.

2. Improved side-rectifier configuration with heat integration

Following the initial idea of (Agrawal, 2000a, 2000b) an improved side-rectifier configuration with heat integration is derived in a sequence of steps, starting from the direct split configuration, as illustrated in Figure 1.

Figure 1: Transformation from direct split sequence over the thermally-coupled side rectifier to a heat-integrated LOT side-rectifier (HI-LOT-SR) configuration.
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First, the direct split is converted to a thermally coupled side-rectifier, by an initial heat transfer of the reboiler of the first column (step 1) and a consecutive replacement of the reboiler by means of the bidirectional transfer of liquid and vapor (step 2). Subsequently the side-rectifier is modified to a LOT configuration, by exchanging the bidirectional transfer with a one-sided liquid transfer from the first to the second column, while extending the second column with an additional stripping section (step 3). Finally, a pump and heat exchanger are introduced into the liquid side stream in order to modify the operating pressure ($p_2$) of the second column (step 4). Pressure $p_2$ is determined such that the boiling temperature of the intermediate boiling product B is raised sufficiently above the boiling temperature of the heavy boiling product C at the operating pressure of the first column ($p_1$), enabling direct heat integration between both columns.

According to Agrawal (2000a), this heat-integrated LOT side-rectifier (HI-LOT-SR) configuration could also be implemented in a consecutive column shell, when locating the second column on top of the first one (step 5).

3. Shortcut-based screening of alternative process configurations

In order to evaluate the potential benefits of the introduced HI-LOT-SR configuration, its performance has to be compared with alternative process configurations. For this purpose a shortcut-based screening method, developed in previous work (Skiborowski, 2018), is applied and extended, in order to include the HI-LOT-SR configuration. The initially developed algorithmic framework enables the evaluation of the minimum energy requirement (MED) of the simple column configurations (direct, indirect and intermediate split), six thermally coupled versions of these simple configurations, a heat integrated alternative for each of the simple configurations, as well as six configurations that consider MVR for either one or both columns in the direct and indirect split. Together with the LOT-SR and HI-LOT-SR a total number of 20 process configurations are evaluated by means of the Rectification Body Method (Bausa et al., 1998), while additional flash calculations and parametric optimizations are performed to evaluate the optimal distribution of the medium boiling product in the prefractionator, the distribution of heat loads in the LOT design, as well as the pressure levels in the heat-integrated and MVR designs (Skiborowski, 2018).

4. Economical optimization through MESH-based superstructure models

In order to evaluate the economic performance a MESH-based superstructure model is implemented and solved in GAMS, based on the previously developed superstructure models for simple and energy-integrated distillation processes (Waltermann and Skiborowski, 2019). The resulting mixed-integer nonlinear programming problem is solved in terms of a polythlic solution approach by means of a series of continuously relaxed nonlinear programming problems with the aid of additional nonlinear complementary constraints. The superstructure model for the HI-LOT-SR is a direct extension of the heat-integrated direct split configuration presented by (Waltermann and Skiborowski, 2019), for which an additional side stream is introduced for the first column, which is further connected to the second column, passing through the intermediate pump and heat exchanger, instead of the bottoms product. The latter is supposed to provide the heavy boiling product with the required purity specifications, as illustrated in Figure 1. The respective equation-oriented model for the superstructure and the economic model are described in further detail by (Waltermann et al., 2019; Waltermann and Skiborowski, 2019).
5. Case study

In the scope of the current study the separation of a zeotropic mixture of benzene, toluene and ethylbenzene is investigated. 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. While the separation of this mixture, with a feed composition of 70 mol% benzene, 20 mol%, toluene and 10 mol% ethylbenzene was considered in the previous development of the shortcut screening approach (Skiborowski, 2018), the extended algorithmic framework is now used to evaluate potential feed compositions, for which the HI-LOT-SR provides potential MED savings in respect to all considered process configurations. Furthermore, an economic evaluation of the HI-LOT-SR is performed for the feed composition for which the largest MED savings are determined.

5.1. Shortcut-based screening

The MED of the 20 considered process configurations is evaluated for 171 feed compositions, resulting from an equidistant scattering of the composition space with variations in single component compositions of 5 mol%. Despite an energy conversion factor of 2 and isentropic and mechanical efficiencies of 80% and 90%, the MVR configurations provide generally the lowest MED. However, when considering the depreciation of the necessary compressor in the calculation of an estimate of the annual operating costs (AOC), MVR configurations are not the favorable choice for any of the feed compositions. Therefore, the following evaluation of the MED is first limited to the 14 configurations, excluding the MVR configurations. The results of this evaluation are illustrated in Figure 2, which indicates by means of different symbols, which process configuration provides the lowest MED for a specific feed composition.

Figure 2: Illustration of favorable process configurations in terms of MED for different feed compositions (symbols indicate favorable process configuration at the specific feed composition).

While partially and fully thermally coupled configurations are preferred for high concentrations of benzene and low concentrations of toluene, heat-integrated direct split and prefractionator configurations are preferred for medium to high concentrations of toluene and low concentrations of ethylbenzene. The HI-LOT-SR provides the lowest MED for all feed compositions with medium to high concentrations of ethylbenzene. It has the lowest MED for 47% of the evaluated feed compositions, allowing for a
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reduction of more than 20%(30%) in respect to the best alternative configuration for 38(8) of the considered feed composition, with 34.4% saving potential for a feed composition of 15 mol% benzene, 15 mol%, toluene and 70 mol% ethylbenzene.

For the separation of a feed stream of 10 mol/sec and this feed composition, the required MED and the according AOC estimates of all 20 considered process configurations are illustrated in Figure 3. As highlighted, the fully thermally coupled DWC is the next best configuration in terms of MED, apart from the MVR configurations. Yet, it requires 52% more energy, which translates into similar savings in AOC, assuming that both processes are heated with the same high pressure steam.

Figure 3: Illustration of single process performance for the selected feed composition in terms of MED (left) and estimated AOC (right)

5.2. Economic optimization

For further comparison the HI-LOT-SR configuration and the fully thermally coupled DWC are evaluated on the basis of an economically optimized design, making use of the aforementioned superstructure optimization approach (Waltermann and Skiborowski, 2019, 2017). The results are illustrated in Figure 4, considering a depreciation period of 5 years, an interest rate of 6% and an annual operating time of 8000h.

Figure 4: Illustration of the results of the economic process optimization.
All products are required to be of 99.9 mol% purity. Given these assumptions, the DWC is still the most economic process, with a significantly lower investment. Yet, the rigorous design optimization confirms the potential energy savings determined by means of the shortcut screening, which however do not directly translate to AOC savings, since 20 bar steam is required for the reboiler of the second column in the HI-LOT-SR configuration, while 10 bar steam suffices for the DWC. Although the DWC is deemed economically superior under the current assumptions, the HI-LOT-SR configuration becomes more attractive in case of higher depreciation and utility costs.

6. Conclusions

The combination of thermal coupling and heat integration, enabled by the LOT modification, provides a promising option for further improvement of the energy efficiency of distillation processes. The comparative evaluation of multiple energy integrated process configurations highlights the significant improvement potential offered by the considered HI-LOT-SR configuration. The outlined combination of a shortcut-based screening and a subsequent economic optimization enables a time-efficient and case-specific evaluation of possible applications as well as a detailed economic comparison of the most promising options. As illustrated in the current case study such evaluation is of significant importance in order to determine the most effective process configuration for a specific application and economic scenario.

References

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