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Simultaneous Heat and Mass Flow Optimization of a Distillation Column Applying the FluxMax Approach

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The transition from fossil to renewable resources requires energy-efficient technologies and approaches in chemicals production. Critical aspects for energy and resource consumption are distillation columns due to their high energy demand and low energy efficiency. Therefore, the optimal design of distillation columns is crucial for increasing the overall energy efficiency. In this contribution, we present the application of the FluxMax approach to the separation section of the methanol synthesis. The FluxMax approach enables the simultaneous flux optimization and heat integration of chemical processes by discretization of the thermodynamic state space. As a consequence, the process-based nonlinearities are effectively decoupled from the subsequent flow optimization problem. The distillation process is represented by the elementary processes mixing, heating, cooling, and flash separation. By simultaneously considering heat integration in the optimization problem, each tray of the distillation column can be represented by means of the introduced elementary processes. The optimal number of trays and the optimal reflux ratio are direct results of the flux optimization. The FluxMax approach is applied to the methanol–water separation using two different objective functions: energy minimization and tray number minimization. The presented results provide the proof of concept for the use of the FluxMax approach to the synthesis of distillation columns that can be embedded in an overall process optimization.

1. Introduction

In order to achieve the settled climate targets, the chemical industry is required to reduce the carbon dioxide emissions drastically. In addition to the substitution of raw materials by renewable resources, an increase in resource and energy efficiency would lead to a reduction in emissions. A critical aspect for the energy and resource consumption of chemical processes is the product purification due to the high energy demand and low energy efficiency of distillation columns (Meyer et al., 2018). In particular, the remixing of already separated flows within the column and large temperature differences in the reboiler and condenser lead to large energy losses (Halvorsen and Skogestad, 2018). As a consequence, many publications have been published in recent years aiming to identify energy optimal distillation column designs. Ledezma-Martínez et al. (2018) investigated crude oil distillation systems and showed that a preflash unit can reduce the heating duty. Jiang et al. (2018) compared different process intensification strategies for a multicomponent distillation and explored the possibility of using synergy effects to design energetically and economically efficient distillation systems. A graph-theoretic approach that represents a chemical process as a network of nodes and edges, resulting in a mixed-integer optimization problem, was introduced by Friedler et al. (1992). In another work this concept was used to solve separation-network synthesis problems (Heckl et al., 2010). Further mixed-integer approaches based on surrogate models can be found in literature, that try to overcome challenges caused by dynamic operation (Schäfer et al., 2019) or the need for global optimality (Keßler et al., 2019). In contrast, Holiastos and Manousiouthakis (2004) introduced an infinitely dimensional linear programming approach to identify globally optimal distillation network designs.
The recently introduced FluxMax approach (Schack et al. 2019) also enables the optimization of chemical processes across different length scales while avoiding binary decision variables. The key features of the FluxMax are the simultaneous flux optimization and heat integration as well as the effective decoupling of process-based nonlinearities through discretization of the thermodynamic state space. In this sense, the

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methodology of the network approach, which was introduced and further developed in Schack et al. (2016) and Schack et al. (2018), on the one hand, and the decoupling strategy applied in Liesche et al. (2018), on the other hand, can be seen as the basis of the FluxMax approach.
In the present contribution, the FluxMax approach is applied to the separation of methanol–water mixtures by distillation. The elementary processes of mixing, heating, cooling, and flash separation are introduced for the representation of single column trays, which enables the modeling of the entire distillation column (Figure 1).

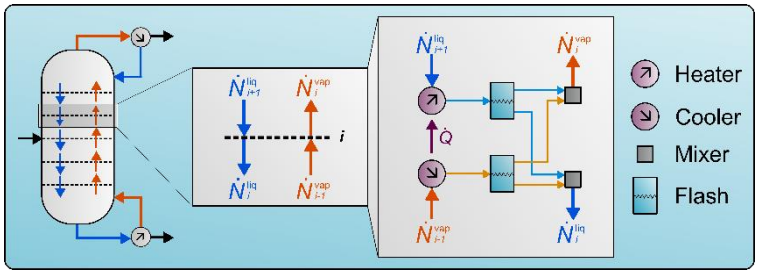

Figure 1: Illustration of the overall distillation process and single tray fluxes

2. FluxMax approach

The key idea of the FluxMax approach is to decouple process-based nonlinearities from the subsequent flow optimization problem by discretization of the thermodynamic state space. The introduction of nodes allows the representation of a chemical process as a directed graph. The FluxMax approach can be divided into three steps as shown in Figure 2: i) discretization of the thermodynamic state space, ii) modeling of the transitions between discrete state points, and iii) simultaneous flow optimization and heat integration.
Using the methanol synthesis process as an example, the FluxMax approach has so far been successfully applied to different levels of the chemical process hierarchy: on the i) plant level for the systematic analysis of different feedstock and energy sources (Schack et al., 2018), ii) process level for identifying energy-optimal overall process configurations that outperform configurations identified in a sequential procedure (Schack et al., 2019), iii) process unit level for optimizing the compressor cascade and reactor part (Liesche et al., 2018). Furthermore, the FluxMax approach was applied to the high energy consuming hydrogen cyanide process and it was shown that a combination of different reactor and recycling strategies strongly reduces the variable cost and increases the resource efficiency (Liesche et al., 2019).

2.1 Digraph representation of distillation process

In case of an isobaric distillation process, the thermodynamic state space is described by the thermodynamic coordinates temperature T and molar compositions x_α of the components α. Three types of nodes are introduced: thermodynamic substance nodes (TSN) $\mathrm{M}_i \in \mathcal{M}$, elementary process nodes (EPN) $\mathrm{E}_j \in \mathcal{E}$, and utility nodes (UN) $\mathrm{U}_l \in \mathcal{U}$, where $\mathcal{M}, \mathcal{E}$ and $\mathcal{U}$ denote the sets of all TSNs, EPNs, and UNs, respectively.

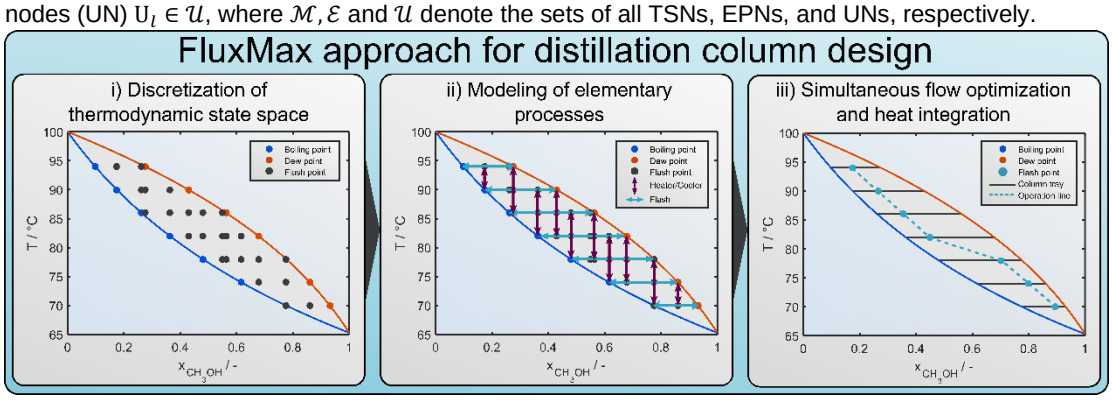

Figure 2: Illustration of FluxMax approach for distillation column design

A TSN is a discrete state point in the thermodynamic state space $(T, \mathbf{x})$ and thus corresponds to a specific chemical mixture at distinct temperature and composition. The transition from one TSN M_i to another M_{i+1} indicates a change of at least one thermodynamic coordinate, which is facilitated by the EPN E_j. For each EPN, a stoichiometric equation with generalized stoichiometric coefficients $\chi_{(\mathrm{E}_j)}^{(\mathrm{M}_i)}$ is introduced, which expresses the

molar change of M_i during its transition through E_j. According to Figure 2, two types of EPN are required, corresponding to the elementary processes of heating/cooling and flash separation. It is important to mention that no unique EPN is required for the mixing process as only mixtures with identical thermodynamic coordinates are mixed. Thus the TSNs itself can be considered as mixers. The stoichiometric coefficients for heating and cooling equal unity and minus unity ($\mathrm{M}_1 \longrightarrow \mathrm{M}_2$), respectively, as the number of moles remains constant. The stoichiometric equation for each elementary flash separation process S_j is given as follows:

$$\mathrm{M}_1 \longrightarrow \chi_{(\mathrm{S}_j)}^{(\mathrm{M}_2)}\mathrm{M}_2 + \chi_{(\mathrm{S}_j)}^{(\mathrm{M}_3)}\mathrm{M}_3 \quad \forall\, \mathrm{S}_j \in \mathcal{E} \tag{1}$$

The stoichiometric coefficients $\chi_{(\mathrm{S}_j)}^{(\mathrm{M}_i)}$ are determined by the following equation system, where $x_{\alpha,\mathrm{F}}$ denotes the molar composition of α of the flash inlet flux, and $x_{\alpha,\mathrm{B}}$, $x_{\alpha,\mathrm{D}}$ denote the corresponding compositions at the boiling (B) and dew (D) curve at flash temperature:

$$x_{\alpha,\mathrm{F}} = \chi_{(\mathrm{S}_j)}^{(\mathrm{M}_2)} x_{\alpha,\mathrm{B}} + \chi_{(\mathrm{S}_j)}^{(\mathrm{M}_3)} x_{\alpha,\mathrm{D}} \tag{2}$$

$$1 = \chi_{(S_j)}^{(M_2)} + \chi_{(S_j)}^{(M_3)} \tag{3}$$

In addition, a generalized process extent number (PEN) $\dot{\Gamma}_{(\mathrm{E}_j)}$ is introduced for each EPN, which serves as measure of the process extent. Since $\dot{\Gamma}_{(\mathrm{E}_j)}$ equals zero if E_j is inactive, the PEN also determines active EPNs in the subsequent optimization problem. The third class of nodes, the UNs U_l, are introduced for two reasons. First, the UNs provide the external heating and cooling duty at predefined temperature levels. Secondly, the UNs enable simultaneous heat integration as an integral part of the optimization problem by introducing additional inequality constraints as described in 2.3.

2.2 Conservation laws of the distillation process

Steady state behavior is assumed, which results in no accumulation of mass and/or energy within the nodes. Table 1 shows the mass- and energy balances for the three nodes introduced above.

Table 1: Conversion laws for introduced nodes

Node	Mass balances	Energy balances
TSN $\forall\, \mathrm{M}_i \in \mathcal{M}$	$0 = \sum_{E_j \in \mathcal{E}} \mathrm{sgn}\left(\chi_{(\mathrm{E}_j)}^{(\mathrm{M}_i)}\right) \dot{N}_{(\mathrm{E}_j)}^{(\mathrm{M}_i)} + \dot{N}_{\mathrm{ext,in}}^{(\mathrm{M}_i)} - \dot{N}_{\mathrm{ext,out}}^{(\mathrm{M}_i)}$	-
EPN $\forall\, \mathrm{E}_j \in \mathcal{E}$	$0 = -\mathrm{sgn}\left(\chi_{(\mathrm{E}_j)}^{(\mathrm{M}_i)}\right) \dot{N}_{(\mathrm{E}_j)}^{(\mathrm{M}_i)} + \chi_{(\mathrm{E}_j)}^{(\mathrm{M}_i)} \dot{\Gamma}_{(\mathrm{E}_j)}$	$0 = \sum_{\mathrm{U}_l \in \mathcal{U}} \dot{Q}_{(\mathrm{E}_j)}^{(\mathrm{U}_l)} - \sum_{\mathrm{U}_l \in \mathcal{U}} \dot{Q}_{(\mathrm{U}_l)}^{(\mathrm{E}_j)} + \varphi_{(\mathrm{E}_j)}^{\mathrm{out}} \dot{\Gamma}_{(\mathrm{E}_j)} - \varphi_{(\mathrm{E}_j)}^{\mathrm{in}} \dot{\Gamma}_{(\mathrm{E}_j)}$
UN $\forall\, \mathrm{U}_l \in \mathcal{U}$	-	$0 = \sum_{\mathrm{U}_l \in \mathcal{U}} \dot{Q}_{(\mathrm{U}_l)}^{(\mathrm{E}_j)} - \sum_{\mathrm{U}_l \in \mathcal{U}} \dot{Q}_{(\mathrm{E}_j)}^{(\mathrm{U}_l)} + \dot{Q}_{(\mathrm{U}_l)}^{\mathrm{ext,in}} - \dot{Q}_{(\mathrm{U}_l)}^{\mathrm{ext,out}}$

The TSNs distribute mixtures with the same thermodynamic state within the chemical process network. Consequently, a TSN is connected by internal mass fluxes $\dot{N}_{(\mathrm{E}_j)}^{(\mathrm{M}_i)}$ corresponding to the input- or output fluxes of EPNs, and by external fluxes that correspond to initially provided reactants or the final product. No energy balances are required for TSNs as the thermodynamic state of all fluxes interacting with M_i is by definition identical, i.e. a mixture of the same composition but different temperature results in different TSNs.
The chemical transition within the thermodynamic state space takes place via the EPNs. As a result, energy balances are formulated in addition to mass balances. The molar ratio of outlet and inlet fluxes is determined by the generalized stoichiometric coefficient $\chi_{(\mathrm{E}_j)}^{(\mathrm{M}_i)}$ and the extent of the elementary process is described by the generalized process extent number (PEN) $\dot{\Gamma}_{(\mathrm{E}_j)}$. The heat fluxes $\dot{Q}_{(\mathrm{E}_j)}^{(\mathrm{U}_l)}$ and $\dot{Q}_{(\mathrm{U}_l)}^{(\mathrm{E}_j)}$ connect an EPN to an UN and are dependent on the specific heating duty $\varphi_{(\mathrm{E}_j)}^{\mathrm{in}}$ or specific cooling duty $\varphi_{(\mathrm{E}_j)}^{\mathrm{out}}$. These specific duties are calculated a priori, e.g. by nonlinear equations of state. While the superscripts of the fluxes denote the origin node, the subscript denotes the destination node.
The utility nodes do not interact with mass fluxes, but only with heat fluxes. In addition to the external fluxes corresponding to the external heating $\dot{Q}_{(\mathrm{U}_l)}^{\mathrm{ext,in}}$ and cooling fluxes $\dot{Q}_{(\mathrm{U}_l)}^{\mathrm{ext,out}}$, the internal fluxes $\dot{Q}_{(\mathrm{U}_l)}^{(\mathrm{E}_j)}$ and $\dot{Q}_{(\mathrm{E}_j)}^{(\mathrm{U}_l)}$ provide the heating and cooling internally, as presented in the following section.

2.3 Heat integration

In this work the heat integration model derived in Schack et al. (2019) is used. In addition to the external heating and cooling supply, the UNs also enable heat integration. Therefore, an UN is introduced for each discrete flash temperature corresponding to a single column tray, as shown in Figure 3. If no minimum temperature difference is considered – justified by the direct mixing of hot and cold flows in distillation columns – two inequalities are sufficient to limit the heat fluxes transferred from hot streams to the utilities (Eq(4)) or from utilities to the cold streams (Eq(5)), respectively. Here, $T_i^{\mathrm{util}}, T_{\mathrm{in}}^{(\mathrm{E}_j)}, T_{\mathrm{out}}^{(\mathrm{E}_j)}$ denote the temperatures of *i*-th utility and the inlet and outlet temperatures of the corresponding cold or hot stream. In addition, $\mathcal{K}_m^{\mathrm{util}}$ denotes the *m*-th row of the set of all possible permutations of the interacting utilities $\mathcal{K}^{\mathrm{util}}$ as derived in Schack et al. (2019).

$$0 \leq \frac{T_{\mathrm{in}}^{(\mathrm{E}_j)} - \min\left(T_k^{\mathrm{util}}\right)}{T_{\mathrm{in}}^{(\mathrm{E}_j)} - T_{\mathrm{out}}^{(\mathrm{E}_j)}} \varphi_{(\mathrm{E}_j)}^{\mathrm{out}} \dot{\Gamma}_{(\mathrm{E}_j)} - \sum_{k \in \mathcal{K}_m^{\mathrm{util}}} \dot{Q}_{(\mathrm{U}_l)}^{(\mathrm{E}_j)} \quad \forall\, \mathcal{K}_m^{\mathrm{util}} \tag{4}$$

$$0 \leq \frac{\max\left(T_k^{\mathrm{util}}\right) - T_{\mathrm{in}}^{(\mathrm{E}_j)}}{T_{\mathrm{out}}^{(\mathrm{E}_j)} - T_{\mathrm{in}}^{(\mathrm{E}_j)}} \varphi_{(\mathrm{E}_j)}^{\mathrm{in}} \dot{\Gamma}_{(\mathrm{E}_j)} - \sum_{k \in \mathcal{K}_m^{\mathrm{util}}} \dot{Q}_{(\mathrm{E}_j)}^{(\mathrm{U}_l)} \quad \forall\, \mathcal{K}_m^{\mathrm{util}} \tag{5}$$

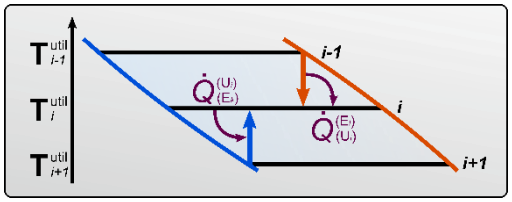

Figure 3: Illustration of heat integration model

2.4 Objective functions

All balances and inequalities presented in 2.2 and 2.3 are linear in terms of the fluxes $\boldsymbol{\varphi} = \left(\dot{\mathbf{N}}, \dot{\mathbf{Q}}, \dot{\boldsymbol{\Gamma}}\right)$ and serve as constraints in the optimization problem. The general form of an optimization problem with linear constraints is given in Eq(6). Herein, $\mathbf{A}$ and $\mathbf{b}$ denote the coefficient matrix and solution vector resulting from the conservation laws (Table (1)) and inequalities (Eqs.(4)-(5)). The lower $\boldsymbol{\varphi}_{\mathrm{lb}}$ and upper bounds $\boldsymbol{\varphi}_{\mathrm{ub}}$ limit the fluxes and are set with regard to the chosen scenario.

$$\begin{aligned} \min_{\boldsymbol{\varphi}} \quad & f(\boldsymbol{\varphi}) \\ \text{s.t.} \quad & \mathbf{A}\boldsymbol{\varphi} \leq \mathbf{b} \\ & \boldsymbol{\varphi}_{\mathrm{lb}} \leq \boldsymbol{\varphi} \leq \boldsymbol{\varphi}_{\mathrm{ub}} \end{aligned} \tag{6}$$

Two different objective functions f are introduced in the following: minimization of i) energy, and ii) number of column trays. The first objective function seeks to identify energy optimal column designs and minimize the sum of external heating and cooling duties:

$$f^{\mathrm{I}}(\boldsymbol{\varphi}) = \sum_{\mathrm{U}_l \in \mathcal{U}} \dot{Q}_{(\mathrm{U}_l)}^{\mathrm{ext,in}} + \sum_{\mathrm{U}_l \in \mathcal{U}} \dot{Q}_{(\mathrm{U}_l)}^{\mathrm{ext,out}} \tag{7}$$

In contrast to the first objective function f^{I}, which seeks for energy efficiency, the minimization of the number of trays can be seen as a measure of the capital cost of the column and thus as an economic efficiency. The number of trays is minimal if the liquid reflux stream from the condenser to the top tray is maximized. According to the FluxMax approach, this liquid reflux stream corresponds to the sum of all liquid fluxes that are heated at the lowest flash temperature under consideration $\dot{N}_{(\mathrm{D}_j)}^{\mathrm{liq,top}}$ by means of the heaters $\mathrm{D}_j \in \mathcal{E}$.

$$f^{\mathrm{II}}(\boldsymbol{\varphi}) = -\sum_{\mathrm{D_j} \in \mathcal{E}} \dot{N}_{(\mathrm{D}_j)}^{\mathrm{liq,top}} \tag{8}$$

A key parameter of distillation columns is the reflux ratio r, which is defined as ratio between liquid reflux stream from the condenser and the total top product stream $\dot{N}_{\mathrm{top}}$:

$$r = \sum_{\mathrm{D_j} \in \mathcal{E}} \dot{N}_{(\mathrm{D}_j)}^{\mathrm{liq,top}} / \dot{N}_{\mathrm{top}} \tag{9}$$

3. Results

In the case study under consideration, a 50/50 feed mixture of methanol and water is to be separated at a constant pressure of $p = 1\ \mathrm{bar}$. The molar fraction of methanol is fixed at $x_{\mathrm{CH_3OH}}^{\mathrm{top}} = 0.926$ at the top of distillation column and $x_{\mathrm{CH_3OH}}^{\mathrm{bot}} = 0.167$ at the bottom, and the temperature conditions are as follows: $T^{\mathrm{feed}} = 80\ °\mathrm{C}$; $T^{\mathrm{top}} = 70\ °\mathrm{C}$; $T^{\mathrm{bot}} = 90\ °\mathrm{C}$. The feed and product specifications are shown in Figure 4 as magenta and green dots. The thermodynamic state space is discretized within the feasible region determined by the vapor-liquid equilibrium. In the following, only a coarse discretization of the flash temperatures – 2 °C-steps between top and bottom temperature – is chosen to better illustrate the optimal pathway. Ideal conditions are assumed to calculate the specific heating duty $\varphi_{(\mathrm{E}_j)}^{\mathrm{in}}$ or specific cooling duty $\varphi_{(\mathrm{E}_j)}^{\mathrm{out}}$ by evaluating the enthalpy differences between discrete TSNs. Figure 4 shows the optimal pathway along the thermodynamic state space for the defined case study depending on the selected objective function

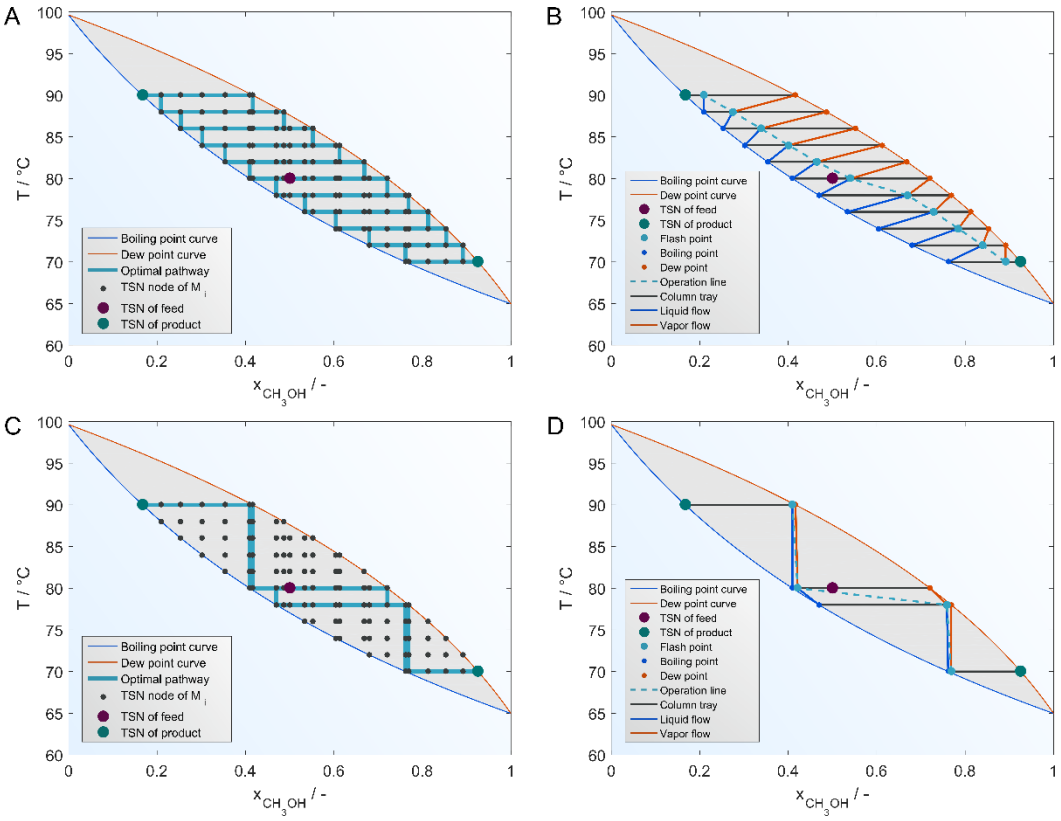

Figure 4: Optimal pathway within the thermodynamic state space for the two objective functions

The left-hand sides (Figure 4 A and C) show the optimal flux network resulting directly from the optimization and the right-hand sides (Figure 4 B and D) are obtained by calculation of the mixing point of each tray that result from all fluxes entering a distinct tray. The results for the minimization of the total energy duty (Eq(7)) are illustrated only once in Figure 4 A and B. It can be seen that the total energy duty is minimized if the number of separation trays equals the maximum number of possible flash steps (9+2). As a consequence, the operating line (cyan dashed line) is near the boiling point curve in the stripping section of the column and near the dew point curve in the rectifying section. The total energy duty is $35.7\ \mathrm{kW/mol_{feed}}$ and the reflux ratio equals 0.27. In contrast, the minimization of the trays leads to four separation steps: 2 trays, 1 reboiler and 1 condenser. In this case, however, the separation requires a reflux ratio of 22.45 and a total energy duty of $328.2\ \mathrm{kW/mol_{feed}}$. The resulting operation line has the shape of a zigzag curve with alternating flash points close to the boiling point and dew point curve.

While the minimization of the energy duty corresponds to minimizing the operating cost, the minimization of trays seeks for a compact column design and thus corresponds to capital cost minimization. Therefore, in a real technical application, an adequate trade-off must be found between the two conflicting objectives, which can be easily assessed by selecting the total cost as an objective function of the FluxMax approach.

Table 2: Overview of the results obtained for the two different objective functions

Objective function	Heating duty / kW	Cooling duty / kW	Number of trays	Reflux ratio
Energy minimization	20.2	15.0	9+2	0.27
Tray minimization	166.7	161.5	2+2	22.45

4. Conclusion

This paper presents the application of the FluxMax approach to the distillation design problem of the methanol-water separation. The process-based nonlinearities are decoupled from the optimization problem by discretization of the thermodynamic state space and the representation of the distillation process by three elementary processes: mixing, heating/cooling, and flash separation. As a consequence of the simultaneous consideration of heat integration through the introduction of inequality constraints, the optimal column design can be identified. Two different objective functions were used to illustrate the versatility of the FluxMax approach: minimization of i) energy duty, and ii) number of trays.

Since the selected objective functions correspond to extreme cases, the objective functions will be extended in our future work to account for industrial applications. In chemical processes, the separation is usually not the main step, but embedded into an entire process. This contribution can thus be used to optimize the entire production process by introducing further elementary processes such as reaction and compression. In particular, the consideration of different pressures allows not only the identification of single distillation columns, but also complex distillation sequences.

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