Kaibel Column: Modeling, Optimization, and Conceptual Design of Multi-product Dividing Wall Columns

E. Soraya Rawlings[a, *], Qi Chen[b], Ignacio E. Grossmann[b], and Jose A. Caballero[c]

[a]Departamento de Ingenieria Quimica, Instituto Tecnologico de Celaya, 600 Antonio Garcia Cubas Esq. Av. Tecnologico, Celaya 38010, Mexico
[b]Department of Chemical Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh 15213, USA
[c]Departamento de Ingenieria Quimica, Universidad de Alicante, Carretera San Vicente S/N, Alicante 03690, España
[*]Corresponding author: E. Soraya Rawlings, sorayadex@gmail.com

Abstract

In this work, we present the modeling, optimization, and conceptual design of a dividing wall column for the separation of four products, commonly referred to in the literature as a Kaibel column. For its solution, we propose and validate a rigorous tray-by-tray model, followed by its reformulation to include a mixed-integer nonlinear programming and a general disjunctive programming formulation to respond to the conceptual design problem attached to these complex configurations. Considering the validated model and the two formulations, the Kaibel column is solved, obtaining four high-purity products and new optimal tray locations for the feed and two side product streams, when the mixed-integer nonlinear programming formulation is applied. The use of these optimally located side streams showed reductions in the energy consumption when compared to cases were non-optimal fixed tray locations are used. When the general disjunctive programming problem was solved, the minimum number of trays needed in the main column and dividing wall are obtained, showing a great reduction of the remixing effects in the Kaibel column, and with that, a more energy efficient configuration. The models were coded in Pyomo using the solver IPOPT for the solution of the nonlinear programming problem, the solver Bonmin for the solution of the mixed-integer nonlinear programming problem, and GDPopt for the solution of the general disjunctive programming optimization problem.

Keywords: Kaibel Column, Dividing Wall Columns, Nonlinear Programming Optimization, Mixed Integer Nonlinear Programming Optimization, General Disjunctive Programming.

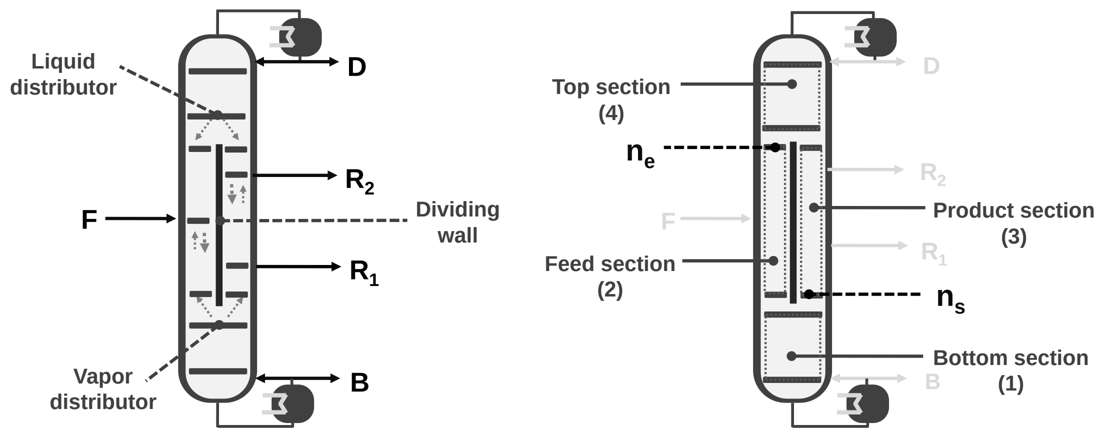
1 Introduction

Distillation is a well known separation process that consumes 40% of the total processing energy in the United States alone (U.S. Department of Energy, 2001). Since the use of distillation columns is unlikely to change, at least for existing plants, process intensification appears as a promising option to optimize these processes by reducing their energy consumption, as its main goal. In separation processes, this intensification has implied the creation of new distillation designs that allow improved separations, especially for mixtures with three or more components (Yildirim et al., 2011). Among these intensified column designs, we find the Petlyuk configuration (Petlyuk et al., 1965), which with further integration and modifications were identified as dividing wall columns (DWC). This column, created by the addition of a wall that physically splits the internal trays of the column in two sections, has proven to be more energy efficient and thus more sustainable than their continuous counterpart, generating savings up to 30 % in energy consumption and savings in capital and investment costs (Dejanović et al., 2010). Although its construction and control still represent a challenging but doable task (Kiss and Baldea, 2011; Gomez-Castro et al., 2008), it has found its use in industry with successful results (Yildirim et al., 2011).

Among the DWCs, different configurations have been proposed depending mainly on the number of components that are separated or the position and number of dividing walls added to the internal trays of the column. A Kaibel column (KC) (Kaibel, 1987), as one of these DWC configurations, is a promising option since it is able to separate more than three products within one single column, replacing a typical distillation sequence of two, three or more distillation columns (Kiss et al., 2012). A detailed scheme of this column is given in Figure 1(a). Even though the KCs have been simulated using commercial software and optimized with the use of external optimization algorithms (Qian et al., 2016; Tututi-Avila et al., 2017), no validated model has been reported for its simulation or optimization. A preliminary version of this work, including a proposed model and the NLP optimization of a KC, is given in Lopez-Saucedo et al. (2018).

The optimization of KCs is not an easy and straightforward task to perform, since it involves not only a complex mathematical model to predict the behavior of the separation in the column, it also involves the selection of a large number of parameters for its design. These not only include the identification of the best intensified configuration to perform a specific task, it also involves the specification of the number of trays and feed and side product streams location that minimize the investment and operating costs. The nonlinear programming (NLP) optimization of KCs is used for the selection of the continuous variables, yielding a performance evaluation (such as operating conditions and energy consumption in the column), but with no design decisions. For the solution of the conceptual design problem involving continuous distillation columns (CDC), and for the optimal selection of their design parameters, two major formulations involving continuous and binary variables have been proposed in the literature: a mixed-integer nonlinear programming (MINLP) model that involves binary variables with the values of "0" or "1" related to the existence of trays or flows in the column (Viswanathan and Grossmann, 1990), and a general disjunctive programming (GDP) model that uses disjunctions to define whether trays exist or not in the column. These two formulations have been successfully applied to the conceptual design of CDCs (Ghouse et al., 2018; Caballero et al., 2005; Barttfeld et al., 2003, 2005; Yeomans and Grossmann, 2000; Jackson and Grossmann, 2001), but there is no reference in the literature of their use for the conceptual design of intensified configurations, such as multi-product DWCs or KCs.

In this paper, we propose and validate a rigorous tray-by-tray model for the optimization and conceptual design of a Kaibel column. To validate the model, we simulate a multi-product DWC, followed by the performance study and optimal design of the KC for the separation of four high-purity products from a methanol-ethanol-propanol-butanol feed mixture. For the performance study, we first solved an NLP optimization problem with fixed tray locations, followed by the solution of the MINLP formulation with fixed number of trays and variable side streams locations to optimally locate a side feed and two product side outlets in the internal trays of the dividing



(a) Kaibel column.

(b) Main sections in the Kaibel column.

Figure 1: Kaibel column and its main sections.

wall. For the GDP formulation, the proposed model is reformulated and solved to determine the minimum number of trays needed in the dividing wall and main column to achieve the desired separation. The problem statement is presented in Section 2, while the rigorous tray-by-tray model for the KC, including the MINLP and GDP model reformulations are explained in detail in Section 3. The case studies are given in Section 4, while the results for the model validation, MINLP and GDP formulations are given in Section 5. Finally, the conclusions are presented in Section 6.

2 Problem Statement

In general, the optimization problem is stated as follows. Given is a feed mixture of NC components with known composition and temperature that is to be separated into NC high-purity products, the problem is to obtain the optimal location of a side feed and two side product streams and the minimum number of trays of a Kaibel column, while minimizing its capital and operating costs. To accomplish this goal, we examine the following formulations: (a) NLP model with a fixed number of trays and fixed feed and side product locations to optimize the column performance, (b) MINLP model with a fixed number of trays for the main column and variable tray location for the feed and side product streams to determine their optimal location, and (c) GDP model with a set of candidate trays to optimize the number of trays in the column. For their solution, the formulations use the reflux and boilup ratios, the liquid distributor, and the heat duties as the manipulated variables in the system.

3 Model Equations

The modeling of KCs depends mostly on the column design and the complexity of the system to be separated. Different from the number of degrees of freedom in CDCs, KCs have six degrees of freedom: the reflux ratio, the product outlets (bottom, intermediate, and distillate product flowrates), and the liquid and vapor flowrates between the two sections of the dividing wall, controlled by a liquid and vapor distributor on the top and bottom section of the column, respectively. Consider that these KC degrees of freedom are valid when the pressure and tray location for the dividing wall and product outlets are known and fixed.

The steady-state equations governing the KC, represented as a DWC with two side outlets in Figure 1(a), were obtained by modifying the mass and energy balances on the internal trays of a CDC. The tray-by-tray model equations that represent all the continuous variables in the system are presented in detail in Equations 1 to 8, including the mass and energy balances in Equations 1 to 4, the equilibrium equations and summations in Equation 5, the liquid and vapor enthalpies in Equation 6, and other equations, such as the reflux and boilup ratios in Equation 8. This set of equations are considered as the nonlinear constraints in the NLP optimization problem for future comparisons. To organize the model equations, the KC is separated into four main sections as shown in Figure 1(b), with trays counted from bottom to top, with the reboiler as tray 1 and the condenser as tray n_T. The total annual cost function (TAC) in Equation 9 is used as the objective function in the NLP and MINLP optimization problems for the KC. It must be noted that, even though this model describes a KC, it could be easily modified for the solution of different dividing wall configurations by adding or removing the side streams in the model.

Sets

$$\begin{aligned}
&C = \{1, n_C\}\\
&W = \{2, 3\}\\
&J_B = \{1..n_s - 1\}\\
&J_W = \{n_s..n_e\}\\
&J_T = \{n_e + 1..n_T\}\\
&J = J_B \cup J_W \cup J_T
\end{aligned}$$

Mass and energy balances

Bottom section: $j \in J_B$

Reboiler: $j = 1$

$$\begin{aligned}
L_{j+1}\ x_{j+1,c} - V_j\ y_{j,c} - B\ x_{j,c} &= 0,\ \forall c \in C\\
L_{j+1}\ h_{j+1} - V_j\ H_j - B\ h_j + Q_{reb} &= 0
\end{aligned}$$

Vapor distributor: $j = n_s - 1$

$$\begin{aligned}
\textstyle\sum_{w\in W} L^w_{j+1}\ x^w_{j+1,c} - L_j\ x_{j,c} + V_{j-1}\ y_{j-1,c} - \sum_{w\in W} V^w_j\ y_{j,c} &= 0,\ \forall c \in C\\
\textstyle\sum_{w\in W} L^w_{j+1}\ h^w_{j+1} - L_j\ h_j + V_{j-1}\ H_{j-1} - \sum_{w\in W} V^w_j\ H_j &= 0
\end{aligned} \tag{1}$$

Internal trays: $j \in J_B \setminus \{1, n_s - 1\}$

$$\begin{aligned}
L_{j+1}\ x_{j+1,c} - L_j\ x_{j,c} + V_{j-1}\ y_{j-1,c} - V_j\ y_{j,c} &= 0,\ \forall c \in C\\
L_{j+1}\ h_{j+1} - L_j\ h_j + V_{j-1}\ H_{j-1} - V_j\ H_j &= 0
\end{aligned}$$

Feed section: $j \in J_W$

Dividing wall starting tray: $j = n_s$

$$\begin{aligned}
F_j\ x^F_{j,c} + L^2_{j+1}\ x^2_{j+1,c} - L^2_j\ x^2_{j,c} + V^2_{j-1}\ y_{j-1,c} - V^2_j\ y^2_{j,c} &= 0,\ \forall c \in C\\
F_j\ h_F + L^2_{j+1}\ h^2_{j+1} - L^2_j\ h^2_j + V^2_{j-1}\ H_{j-1} - V^2_j\ H^2_j &= 0
\end{aligned}$$

Dividing wall ending tray: $j = n_e$

$$\begin{aligned}
F_j\ x^F_{j,c} + L^2_{j+1}\ x_{j+1,c} - L^2_j\ x^2_{j,c} + V^2_{j-1}\ y^2_{j-1,c} - V^2_j\ y^2_{j,c} &= 0,\ \forall c \in C\\
F_j\ h_F + L^2_{j+1}\ h_{j+1} - L^2_j\ h^2_j + V^2_{j-1}\ H^2_{j-1} - V^2_j\ H^2_j &= 0
\end{aligned} \tag{2}$$

Internal trays: $j \in J_W \setminus \{n_s, n_e\}$

$$\begin{aligned}
F_j\ x^F_{j,c} + L^2_{j+1}\ x^2_{j+1,c} - L^2_j\ x^2_{j,c} + V^2_{j-1}\ y^2_{j-1,c} - V^2_j\ y^2_{j,c} &= 0,\ \forall c \in C\\
F_j\ h_F + L^2_{j+1}\ h^2_{j+1} - L^2_j\ h^2_j + V^2_{j-1}\ H^2_{j-1} - V^2_j\ H^2_j &= 0
\end{aligned}$$

Product section: $j \in J_W$

$$
\begin{array}{rcll}
\multicolumn{4}{l}{\text{Dividing wall starting tray: } j = n_s} \\
L^3_{j+1}\ x^3_{j+1,c} - L^3_j\ x^3_{j,c} - R_{1,j}\ x^3_{j,c} - R_{2,j}\ x^3_{j,c} + V^3_{j-1}\ y_{j-1,c} - V^3_j\ y^3_{j,c} & = & 0, & \forall c \in C \\
L^3_{j+1}\ h^3_{j+1} - L^3_j\ h^3_j - R_{1,j}\ h^3_j - R_{2,j}\ h^3_j + V^3_{j-1}\ H_{j-1} - V^3_j\ H^3_j & = & 0 & \\
\multicolumn{4}{l}{\text{Dividing wall ending tray: } j = n_e} \\
L^3_{j+1}\ x_{j+1,c} - L^3_j\ x^3_{j,c} - R_{1,j}\ x^3_{j,c} - R_{2,j}\ x^3_{j,c} + V^3_{j-1}\ y^3_{j-1,c} - V^3_j\ y^3_{j,c} & = & 0, & \forall c \in C \\
L^3_{j+1}\ h_{j+1} - L^3_j\ h^3_j - R_{1,j}\ h^3_j - R_{2,j}\ h^3_j + V^3_{j-1}\ H^3_{j-1} - V^3_j\ H^3_j & = & 0 & \\
\multicolumn{4}{l}{\text{Internal trays: } j \in J_W \setminus \{n_s, n_e\}} \\
L^3_{j+1}\ x^3_{j+1,c} - L^3_j\ x^3_{j,c} - R_{1,j}\ x^3_{j,c} - R_{2,j}\ x^3_{j,c} + V^3_{j-1}\ y^3_{j-1,c} - V^3_j\ y^3_{j,c} & = & 0, & \forall c \in C \\
L^3_{j+1}\ h^3_{j+1} - L^3_j\ h^3_j - R_{1,j}\ h^3_j - R_{2,j}\ h^3_j + V^3_{j-1}\ H^3_{j-1} - V^3_j\ H^3_j & = & 0 &
\end{array}
\tag{3}
$$

Top section: $j \in J_T$

$$
\begin{array}{rcll}
\multicolumn{4}{l}{\text{Liquid distributor: } j = n_e + 1} \\
L_{j+1}\ x_{j+1,c} - \sum_{w \in W} L^w_j\ x_{j,c} + \sum_{w \in W} V^w_{j-1}\ y^w_{j-1,c} - V_j\ y_{j,c} & = & 0, & \forall c \in C \\
L_{j+1}\ h_{j+1} - \sum_{w \in W} L^w_j\ h_j + \sum_{w \in W} V^w_{j-1}\ H^w_{j-1} - V_j\ H_j & = & 0 & \\
\multicolumn{4}{l}{\text{Condenser: } j = n_T} \\
V_{j-1} y_{j-1,c} - L_j x_{j,c} - D x_{j,c} & = & 0, & \forall c \in C \\
V_{j-1}\ H_{j-1} - L_j\ h_j - D\ h_j - Q_{con} & = & 0 & \\
\multicolumn{4}{l}{\text{Internal trays: } j \in J_T \setminus \{n_e + 1, n_T\}} \\
L_{j+1}\ x_{j+1,c} - L_j\ x_{j,c} + V_{j-1}\ y_{j-1,c} - V_j\ y_{j,c} & = & 0, & \forall c \in C \\
L_{j+1}\ h_{j+1} - L_j\ h_j + V_{j-1}\ H_{j-1} - V_j\ H_j & = & 0 &
\end{array}
\tag{4}
$$

Equilibrium equations and composition summations

$$
\left.\begin{array}{rcl}
y_{j,c} & = & K_{j,c}\ x_{j,c},\ \ \forall c \in C \\
K_{j,c} & = & \gamma_{j,c} \left(P^{sat}{}_{j,c} / P_j \right),\ \ \forall c \in C \\
\sum_{i \in C} y_{j,c} & = & 1 \\
\sum_{i \in C} x_{j,c} & = & 1
\end{array}\right\} \forall j \in J \setminus J_W
$$

$$
\left.\begin{array}{rcl}
y^w_{j,c} & = & K^w_{j,c}\ x^w_{j,c},\ \ \forall c \in C \\
K^w_{j,c} & = & \gamma^w_{j,c} \left(P^{w,sat}_{j,c} / P^w_j \right),\ \ \forall c \in C \\
\sum_{c \in C} y^w_{j,c} & = & 1 \\
\sum_{c \in C} x^w_{j,c} & = & 1
\end{array}\right\} \forall w \in W,\ \forall j \in J_W
\tag{5}
$$

where $\gamma_{j,c}$, $\gamma^2_{j,c}$, and $\gamma^3_{j,c}$ are calculated using NRTL.

Liquid and vapor enthalpy

$$
\begin{array}{l}
\left.\begin{array}{rcl}
h_j & = & f(x_{j,c}, T_j, P_j) \\
H_j & = & f(y_{j,c}, T_j, P_j)
\end{array}\right\} \forall j \in J \setminus J_W \\
\left.\begin{array}{rcl}
h^w_j & = & f(x^w_{j,c}, T^w_j, P^w_j) \\
H^w_j & = & f(y^w_{j,c}, T^w_j, P^w_j)
\end{array}\right\} \forall w \in W,\ \forall j \in J_W \\
\left.\begin{array}{rcl}
h_F & = & f(x_{F,c}, T_F, P_F) \\
H_F & = & f(y_{F,c}, T_F, P_F)
\end{array}\right\} j = n_F
\end{array}
\tag{6}
$$

Other equations

Liquid and vapor distributor:

$$
\begin{array}{lll}
V^w_{n_s-1} = d^w_V\ V_{n_s-1} & \text{with} & \sum_{w \in W} d^w_V = 1 \\
L^w_{n_e+1} = d^w_L\ L_{n_e+1} & \text{with} & \sum_{w \in W} d^w_L = 1
\end{array}
\tag{7}
$$

Internal reflux and boilup ratios:

$$\begin{aligned} rr &= (L_{n_T}/V_{n_T-1}) \\ bu &= (V_1/L_2) \end{aligned} \tag{8}$$

Total Annual Cost function:

$TAC = C_H\ Q_{reb} + C_C\ Q_{con} + \frac{I_R(I_R+1)^{P_L}}{(I_R+1)^{P_L}-1}\ (C_{shell} + C_{int} + C_{HE})$

where $C_H = 0.0091$, $C_C = 0.00228$, $C_{shell} = 44,000$, $C_{int} = 272,000$, and $C_{HE} = 4,500$ (from Peters et al. (2003)).

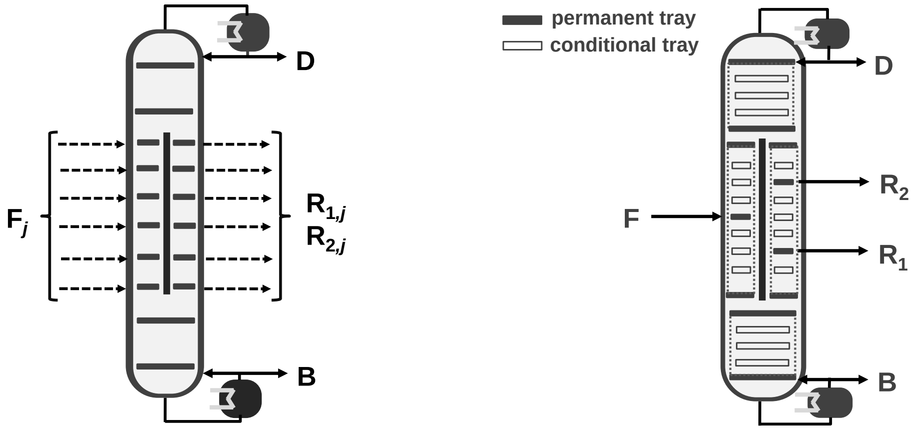
(9)

Since the computational solution of this type of problems depends on the problem structure, the MINLP and GDP formulations involve the reformulation of distillation models for their application. There are different alternative column configurations that can be employed to optimize distillation columns using an MINLP formulation, such as the optimization of the total number of trays or the optimal location of a side feed by considering variable or fixed heat exchange location in the column (Barttfeld et al., 2003). Since we are interested in studying the effects of the location of side streams on the internal sections of the KC, in this work we only consider a configuration with variable tray location for the feed and product streams with fixed condenser and reboiler location, i.e. number of trays in the column. This is shown in Figure 2(a), considering the set of trays in the dividing wall as the candidate trays for the side streams. The MINLP formulation required the addition of new constraints involving the binary variables z_1, z_2, and z_3 to denote the existence of the feed and the two side streams, when they have a value of 1. These new equations are given in Equations 10 and 11.

$$\begin{aligned} &\textstyle\sum_{j\in J_W} F_j \geq F^0 \\ &\textstyle\sum_{j\in J_W} z_{1,j} = 1 \\ &F_j - F^{max}\ z_{1,j} \leq 0\ ,\ \forall j \in J_W \end{aligned} \tag{10}$$

$$\begin{aligned} &\textstyle\sum_{j\in J_W} R_{1,j} \geq R_1^{spec} \\ &\textstyle\sum_{j\in J_W} z_{2,j} = 1 \quad \text{with product constraint } \sum_{j\in J_W} z_{2,j}\ x_{j,3}^3 \geq x_3^{spec} \\ &R_{1,j} - I^{max}\ z_{2,j} \leq 0\ ,\ \forall j \in J_W \\ \\ &\textstyle\sum_{j\in J_W} R_{2,j} \geq R_2^{spec} \\ &\textstyle\sum_{j\in J_W} z_{3,j} = 1 \quad \text{with product constraint } \sum_{j\in J_W} z_{3,j}\ x_{j,2}^3 \geq x_2^{spec} \\ &R_{2,j} - R^{max}\ z_{3,j} \leq 0\ ,\ \forall j \in J_W \end{aligned} \tag{11}$$

The GDP formulation is based on the work by Jackson and Grossmann (2001) and Barttfeld et al. (2003), where a disjunction at each candidate tray describes the existence or absence of the tray. In order to apply this formulation to our proposed KC model and to reduce the number of bilinear terms, we considered individual flows instead of the total flows used in the MINLP formulation. For the modeling of the KC under these new assumptions, we considered the four main sections shown in Figure 1(b), considering that the bottom and top trays for each section are fixed, with the following permanent trays: the reboiler and vapor distributor in the bottom section, the liquid distributor and condenser in the top section, the side feed tray and dividing wall starting and ending tray for the feed side, and the side product trays and dividing wall starting and ending tray in the product section. This is shown in more detail in Figure 2(b). The remaining trays are



(a) Kaibel column representation for MINLP formulation.

(b) Kaibel column representation for GDP formulation.

Figure 2: Kaibel column representations for MINLP and GDP formulations.

considered as candidate trays. The trays in each section are counted from bottom to top, being tray 1 the bottom tray in each section and tray n_P the top tray in each section, where n_P is a specified upper bound for the number of possible trays for each section. For this model, each section has the same number of possible trays. Since the bilinear terms are greatly reduced with the use of individual flows, the liquid and vapor distributor are included in the mass and energy equations. The detailed reformulated model is presented in Equations 12 to 18, including Equation 19 that considers the number of existent trays and operating costs (condenser and reboiler heat duties) in the column. This equation corresponds to the objective function for the GDP formulation. To ensure equal weights to the capital and operating costs, the number of existent trays in Equation 19 is multiplied by a weight coefficient of 1000.

Sets

$C = \{1, n_C\}$
$S = \{1, 4\}$
$W = \{2, 3\}$
$J_1 = J_2 = J_3 = J_4 = \{1..n_P\}$
$J = J_1 \cup J_2 \cup J_3 \cup J_4$

Mass and energy balances

Bottom section: $s = 1$ and $j \in J_1$

$$
\begin{aligned}
&\text{Reboiler: } j = 1\\
&\qquad L_{s,j+1,c} - V_{s,j,c} - B_c = 0, \ \forall c \in C\\
&\qquad \textstyle\sum_{c\in C} \left(L_{s,j+1,c}\, h_{s,j+1,c} - V_{s,j,c}\, H_{s,j,c} - B_c\, h_{s,j,c}\right) + Q_{reb} = 0\\
&\text{Vapor distributor: } j = n_P\\
&\qquad \textstyle\sum_{s\in W} L_{s,1,c} - L_{s,j,c} + V_{s,j-1,c} - \sum_{s\in W} d_V^s\, V_{s,j,c} = 0, \ \forall c \in C\\
&\qquad \textstyle\sum_{c\in C} \left(\sum_{s\in W} L_{s,1,c}\, h_{s,1,c} - L_{s,j,c}\, h_{s,j,c} + V_{s,j-1,c}\, H_{s,j-1,c} - \sum_{s\in W} d_V^s\, V_{s,j,c}\, H_{s,j,c}\right) = 0\\
&\text{Internal trays: } j \in J_1 \setminus \{1, n_P\}\\
&\qquad L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} = 0, \ \forall c \in C\\
&\qquad \textstyle\sum_{c\in C} \left(L_{s,j+1,c}\, h_{s,j+1,c} - L_{s,j,c}\, h_{s,j,c} + V_{s,j-1,c}\, H_{s,j-1,c} - V_{s,j,c}\, H_{s,j,c}\right) = 0
\end{aligned}
\tag{12}
$$

Feed section: $s = 2$ and $j \in J_2$

Dividing wall starting tray: $j = 1$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + d_V^2\ V_{1,n_P,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + d_V^2\ V_{1,n_P,c}\ H_{1,n_P,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned}$$

Side feed: $j = n_F$

$$\begin{aligned} F_c + L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(F_c\ h_{F,c} + L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned}$$

Dividing wall ending tray: $j = n_P$

$$\begin{aligned} d_L^2\ L_{4,1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(d_L^2\ L_{4,1,c}\ h_{4,1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned}$$

Internal trays: $j \in J_2 \setminus \{1, n_F, n_P\}$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned} \tag{13}$$

Product section: $s = 3$ and $j \in J_3$

Dividing wall starting tray: $j = 1$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + d_V^3\ V_{1,n_P,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + d_V^3\ V_{1,n_P,c}\ H_{1,n_P,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned}$$

Side product outlet 1: $j = n_{R_1}$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} - R_{1,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c} - R_{1,c}\ h_{s,j,c}\right) &= 0 \end{aligned}$$

Side product outlet 2: $j = n_{R_2}$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} - R_{2,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c} - R_{2,c}\ h_{s,j,c}\right) &= 0 \end{aligned}$$

Dividing wall ending tray: $j = n_P$

$$\begin{aligned} d_L^3\ L_{4,1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(d_L^3\ L_{4,1,c}\ h_{4,1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned}$$

Internal trays: $j \in J_3 \setminus \{1, n_{R_1}, n_{R_2}, n_P\}$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned} \tag{14}$$

Top section: $s = 4$ and $j \in J_4$

Liquid distributor: $j = 1$

$$\begin{aligned} L_{s,j+1,c} - \textstyle\sum_{s \in W} d_L^s\ L_{s,j,c} + \sum_{s \in W} d_V^s\ V_{s,n_P,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - \sum_{s \in W} d_L^s\ L_{s,j,c}\ h_{s,j,c} + \sum_{s \in W} d_V^s\ V_{s,n_P,c}\ H_{s,n_P,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned}$$

Condenser: $j = n_T$

$$\begin{aligned} V_{s,j-1,c} - L_{s,j,c} - D_c &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(V_{s,j-1,c}\ H_{s,j-1,c} - L_{s,j,c}\ h_{s,j,c} - D_c\ h_{s,j,c}\right) - Q_{con} &= 0 \end{aligned}$$

Internal trays: $j \in J_4 \setminus \{1, n_T\}$

$$\begin{aligned} L_{s,j+1,c} - L_{s,j,c} + V_{s,j-1,c} - V_{s,j,c} &= 0,\ \forall c \in C \\ \textstyle\sum_{c \in C} \left(L_{s,j+1,c}\ h_{s,j+1,c} - L_{s,j,c}\ h_{s,j,c} + V_{s,j-1,c}\ H_{s,j-1,c} - V_{s,j,c}\ H_{s,j,c}\right) &= 0 \end{aligned} \tag{15}$$

Equilibrium equations and composition summations

$$\left.\begin{array}{rcl} y_{s,j,c} & = & K_{s,j,c}\, x_{s,j,c}\ ,\ \ \forall c \in C \\ K_{s,j,c} & = & \gamma_{s,j,c}\left(P^{sat}_{s,j,c}/P_{s,j}\right)\ ,\ \forall c \in C \\ \sum_{c\in C} y_{s,j,c} & = & 1 \\ \sum_{c\in C} x_{s,j,c} & = & 1 \\ & & \\ \multicolumn{3}{l}{\text{with ideal activity coefficients } \gamma_{s,j,c} = 1.} \end{array}\right\}\forall j \in J\ ,\ \forall s \in S \tag{16}$$

Liquid and vapor enthalpy

$$\left.\begin{array}{rcl} h_{s,j,c} & = & f(T_j, P_j) \\ H_{s,j,c} & = & f(T_j, P_j) \end{array}\right\}\forall c \in C\ ,\ \forall j \in J\ ,\ \forall s \in S \tag{17}$$

Other equations

Individual liquid and vapor flowrates:

$$\left.\begin{array}{rcl} L_{s,j,c} & = & L_{s,j}\ x_{s,j,c} \\ V_{s,j,c} & = & V_{s,j}\ y_{s,j,c} \end{array}\right\}\forall c \in C\ ,\ \forall j \in J\ ,\ \forall s \in S$$

Individual side feed and product flowrates:

$$\left.\begin{array}{rcl} F_c & = & F_{total}\ x_{F,c} \\ B_c & = & B_{total}\ x_{1,1,c} \\ D_c & = & D_{total}\ x_{4,n_P,c} \end{array}\right\}\forall c \in C \tag{18}$$

Minimum number of trays equation:

$$n_{min} = (Q_{reb} + Q_{con}) + \omega\ \sum_{s\in S}\ \sum_{j\in J_E}\ n_{s,j} \tag{19}$$

where $\omega = 1000$ and J_E is the set of existent trays.

The candidate trays for each section in the KC are enforced with the use of Boolean variables, as given in the disjunction in Equation 20.

$$\begin{bmatrix} Z_{s,j} \\ f(x_{s,j,c},\ y_{s,j,c},\ V_{s,j,c},\ L_{s,j,c},\ T_{s,j},\ P_{s,j}) = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Z_{s,j} \\ x_{s,j,c} = x_{s,j+1,c} \\ y_{s,j,c} = y_{s,j-1,c} \\ L_{s,j,c} = L_{s,j+1,c} \\ V_{s,j,c} = V_{s,j-1,c} \\ h_{s,j,c} = h_{s,j+1,c} \\ H_{s,j,c} = H_{s,j-1,c} \\ T_{s,j} = T_{s,j+1} \end{bmatrix} \forall j \in J_C,\ \ \forall s \in S \tag{20}$$

where $Z_{s,j}$ are the Boolean variables associated with the tray existence for each section in the column, and $f(x_{j,c}, y_{j,c}, V_{j,c}, L_{j,c}, T_{s,j}, P_{s,j})$ contains the mass and energy balances, equilibrium, enthalpy, and the component and mixture properties equations. When a tray is selected in each section, $Z_{s,j}$ takes the value of “True” (the tray exists) and all the constraints are enforced along with product specifications, but if $Z_{s,j}$ is “False” (or the tray is absent), no changes take place and the flows, compositions, enthalpies, and temperatures entering the tray are set equal to those trays above or below it. For our KC reformulated model, the permanent trays in all the sections are enforced to exist, while the set of candidate trays for each section are: $J_C = \{2..n_P - 1\}$ for the bottom and top sections, $J_C \setminus n_F$ for the feed section, and $J_C \setminus \{n_{R_1}, n_{R_2}\}$ for the product section. We also include logical constraints in order to activate the trays above or below a permanent tray, as given in the logic constraints in Equations 21 and 22. For the feed tray in the feed section these two equations are used, for the trays to exist above and beyond it, while for the bottom, product, and top sections, only the logical proposition in Equation 21 is used.

$$Z_{s,j} \implies Z_{s,j-1} \quad \forall s \in S,\ \forall j \in J_C \tag{21}$$

$$Z_{s,j-1} \implies Z_{s,j} \quad \text{for } s = 2,\ \forall j \in J_C \tag{22}$$

The solution of the two formulations requires not only the specification of certain parameters, such as the number trays, feed location, etc., it also requires an initialization procedure, which consists of the next three steps: (i) a preliminary design of the separation considering a sequence of indirect CDCs to obtain the minimum number of stages with Fenske Equation, (ii) flash calculation for the feed, and (iii) calculation of variable bounds by solving the NLP problem. For the solution of the MINLP formulation, this preliminary phase was applied, followed by the solution of the model Equations 1 to 8 and the objective function in Equation 9, using an MINLP solver. For the GDP formulation, the preliminary phase was also applied, followed by the solution of the model Equations 12 to 18, the disjunctions in Equation 20, and the logical propositions in Equations 21 and 22, considering the objective function in Equation 19.

4 Case Study

The validation of the proposed model and optimal conceptual design of the KC is obtained by performing two different separations. The validation of the model is performed first using the mixture in Case 1, while the optimal conceptual design of the KC using the MINLP and GDP formulation are applied to the mixture in Case 2. The details are explained below.

Case 1. For this case, we perform the separation of a feed mixture of benzene (1), toluene (2), and o-xylene (3) using a DWC, and it is presented first in order to compare and validate the proposed model in Equations 1 to 8 in Section 3. The DWC model was obtained by removing one of the side product streams from the mass and energy balances in Equation 3, and it was simulated using a dummy objective function (objective = 1), with the following product specifications: product flowrates higher than 300 mol/s and final compositions higher than 0.99 for the three components. The operating conditions are given in Table 1. For this case, the location of the side feed, side product stream, and total number of trays for the main column and dividing wall are fixed.

Case 2. For this case, we considered the separation of four high-purity products from a mixture of methanol (1), ethanol (2), propanol (3), and butanol (4) using a KC. For comparison purposes, this column is solved first considering an NLP optimization problem with a fixed total number of trays for the main column, and fixed locations for the feed and side products. The solution of the NLP problem is followed by the MINLP and GDP formulations, with the objective of obtaining the column optimal design parameters. The MINLP formulation is applied to obtain the optimal location of the side feed and two product streams under a fixed total number of trays, while the GDP formulation is solved to obtain the minimum number of trays for the main column and dividing wall, while fixing the location of the feed and side products in the KC. The NLP model and the MINLP and GDP formulations were solved with the operating conditions given in Table

Table 1: Data for Cases 1 and 2.

	Case 1[a]	Case 2		
Operating conditions		NLP	MINLP	GDP
Number of trays	46	58[b]	58[b]	100[c]
Side feed tray	25	31	-	12
Dividing wall starting tray	13	8	8	1
Dividing wall ending tray	36	40	40	25
Side outlet 1 tray	26	18	-	8
Side outlet 2 tray	-	35	-	17
Side feed flowrate in mol/s	1000	$\geq$ 200	$\geq$ 200	200
Side feed temperature in K	358	358	358	358
Vapor distributor to feed section	0.627	0.394	0.394	0.394
Column pressure in bar	0.679 - 0.375	1.20 - 1.05	1.20 - 1.05	1.20
Initial liquid composition				
(1)	0.30	0.25	0.25	0.25
(2)	0.30	0.25	0.25	0.25
(3)	0.40	0.25	0.25	0.25
(4)	-	0.25	0.25	0.25

[a] Data from Ling and Luyben (2010), [b] From Fenske equation
[c] Upper bound for KC, considering an upper bound $n_P = 25$ for each section.

1, including the following final product specifications: product flowrates higher than 50 mol/s and compositions higher than 0.99 for the four components.

The proposed models were written in Python using the package Pyomo (Hart et al., 2011, 2017). IPOPT (Wachter and Biegler, 2006) was used for the solution of the NLP optimization problem, while Bonmin solver (Grossmann et al., 2005) was used to solve the MINLP problem using the algorithm B-Hyb (Hybrid outer-approximation based branch-and-cut algorithm). For the solution of the GDP problem, we used the new logic-based solver GDPopt (Chen et al., 2018).

5 Results

The validation of the proposed model equations is presented in the results in Case 1, followed by the MINLP and GDP formulations results for the conceptual design of KC in Case 2.

Case 1. The DWC simulation results for the separation of benzene, toluene, and o-xylene are presented and compared in Table 2. This comparison between our DWC results with the values from Ling and Luyben (2010) obtained using the commercial software Aspen, shows differences of about 2% between the two columns. These small differences could be due to the constant parameters used for the calculation of the different properties in the system, such as saturation pressure, heat capacity, etc. Considering these small differences as negligible, we can therefore say that the proposed model equations in Section 3 give accurate solutions for multi-product DWC.

Case 2. The NLP optimization results for the KC are given in Table 3, and are presented in order to compare possible benefits of the MINLP solution. The MINLP integer solutions for the KC are also given in Table 3, showing the next optimal locations: the side feed on tray 25 and the side outlets 1 and 2 on trays 16 and 34, respectively. The comparison between the NLP and MINLP solutions shows that, when using the optimally located side streams obtained with the

Table 2: Case 1 results and comparison with commercial software.

Variable	Aspen*	Our Code	**% Error**
Distillate in mol/s	303	302	0.33
Side outlet 1 in mol/s	296	297	-0.33
Bottoms in mol/s	401	401	0
$x_D^{Benzene}$	0.99	0.9927	-0.27
$x_{S1}^{Toluene}$	0.99	0.9902	0
$x_B^{Toluene}$	0.99	0.9908	-0.08
Reboiler duty in MW	35.69	35.43	0.73
Condenser duty in MW	37.52	37.52	0
Reflux ratio (internal)	0.7395[a]	0.7355[b]	0.54
Boilup ratio	0.7020[a]	0.6901[b]	1.69

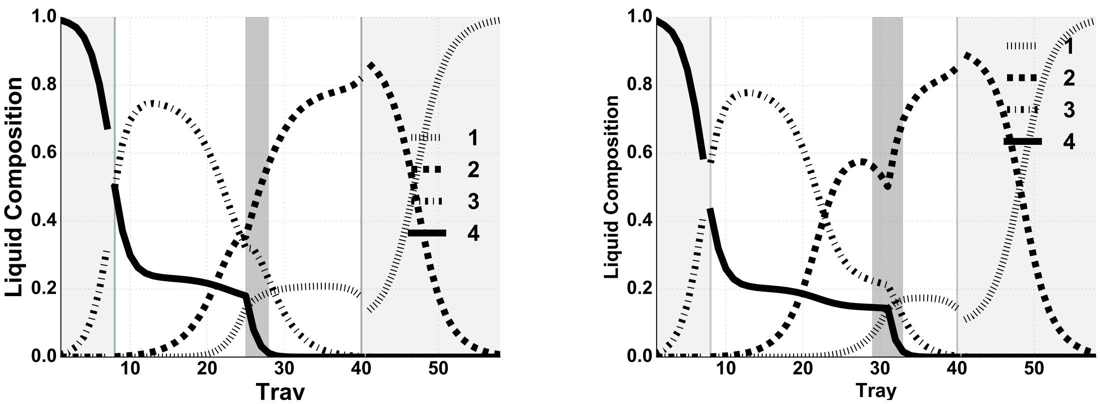
* From Ling and Luyben (2010), [a] Fixed, [b] Calculated.

MINLP formulation, the KC energy consumption in the reboiler is reduced by 11.14%, followed by a reduction of 11.25% in the condenser. These energy savings can be explained by comparing the composition profiles for the prefactionator (or feed side) for the MINLP solution in Figure 3(a) with the NLP solution profiles in Figure 3(b). In Figure 3(a), we observe that the feed mixture enters at tray 25, where small differences between the tray composition and the side feed composition values are observed. Since there are no drastic changes in the composition, this new side feed reduces the mixing losses in the column, thus reducing the energy needed for the separation. This good match is not observed in the NLP composition profiles in Figure 3(b), where the side feed, with smaller composition values, enters on tray 31, reducing the total composition in the tray, and increasing with this the inefficiency in the separation. Smaller reductions on the remixing effects can also be seen in the composition profiles for the product section in Figure 4(a) for the MINLP solution, where a slightly sharper peak is observed, for component 2, when compared to the NLP profile in Figure 4(b). This analysis is consistent with the energy savings observed in the reboiler and condenser in Table 2 for the MINLP solution.

The GDP formulation results are given in Table 4, predicting a total number of trays for the KC of 46 and a dividing wall of 15 trays. This solution reduces the size of the column when compared to the 58-tray KC column used for the NLP and MINLP formulation. This GDP solution increases the efficiency of the separation by decreasing the energy wasted due to remixing effects in all the KC sections. This can be seen in the liquid composition profiles in Figure 5, where sharper peaks for the products in Figure 5(a) are observed, while a better composition match is observed in Figure 5(b) for components 2 and 4 in the side feed tray. Note that the constant composition values are due to the pass through constraints considered in the absent trays.

Table 3: Results for the MINLP formulation using a Kaibel column.

Optimal solutions	NLP	MINLP
Number of trays	58	58
Side feed tray	31	25
Side outlet 1 tray	18	16
Side outlet 2 tray	35	34
Reboiler duty in MW	34.019	30.229
Condenser duty in MW	33.672	29.883
Objective value ($\$/year$)	1,441,823.53	1,286,172.52
Solver	IPOPT	Bonmin (B-Hyb)



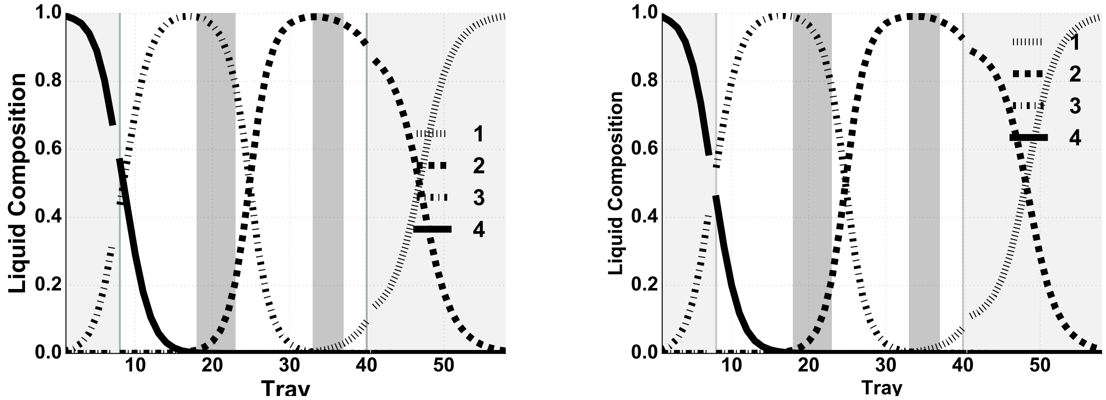
(a) Feed side liquid composition profiles for the MINLP solution.

(b) Feed side liquid composition profiles for the NLP solution.

Figure 3: Liquid composition profiles for the MINLP and NLP solutions for bottoms, feed, and top sections of the Kaibel column. The light gray shaded areas represent the bottom and top sections in the KC, while the darker shaded area represents the side feed F. Components: 1 for methanol, 2 for ethanol, 3 for n-propanol, and 4 for n-butanol.

Table 4: Kaibel column optimal design parameters obtained using the GDP formulation.

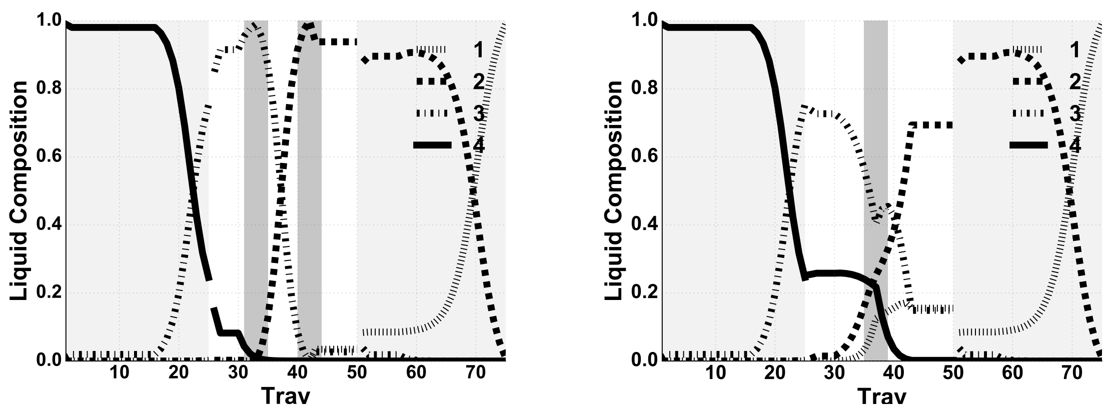
Optimal solutions	GDP
Total number of trays	46
Dividing wall starting tray	12
Dividing wall ending tray	26
Side feed tray	18
Side outlet 1 tray	13
Side outlet 2 tray	22
Solver	GDPopt



(a) Product side liquid composition profiles for the MINLP solution.

(b) Product side liquid composition for the NLP solution.

Figure 4: Liquid composition profiles for the MINLP and NLP solutions for bottoms, product, and top sections of the Kaibel column. The light gray shaded areas represent the bottom and top sections in the KC, while the darker shaded areas represent the product side streams R_1 and R_2. Components: 1 for methanol, 2 for ethanol, 3 for n-propanol, and 4 for n-butanol.



(a) Liquid composition profiles for the product side. The dark gray shaded areas represent the product side streams.

(b) Liquid composition profiles for the feed side. The dark gray shaded area represents the feed.

Figure 5: Liquid composition profiles for the GDP formulation for the Kaibel column. The light gray shaded areas represent the bottom and top sections in the KC. Components: 1 for methanol, 2 for ethanol, 3 for n-propanol, and 4 for n-butanol.

6 Conclusions

In this work, we proposed and validated a rigorous tray-by-tray model for the study of a Kaibel column, while including rigorous MINLP and GDP formulations into its model to determine its optimal conceptual design. In order to validate and determine the accuracy of the proposed model equations, we first compared the results of our model with commercial software results, showing this comparison differences of about 2% under the same operating conditions. Considering this validated model, the Kaibel column is solved applying MINLP and GDP formulations, performing with both the separation of a quaternary feed mixture. With the MINLP optimization, we determined the optimal location of a side feed and two side product streams, showing its comparison to other configurations with no optimally located trays, energy savings of around 11% in the reboiler and condenser. In order to determine the optimal number of trays for the main column and dividing wall, the GDP formulation was applied, showing the results a highly efficient Kaibel column with a reduced number of trays for the main column and dividing wall trays, when compared to the total number of trays used in the MINLP formulation. These results proved how effective these two formulations are to determine the optimal design parameters in dividing wall columns, where their application is assuring a minimization of the energy wasted on remixing effects.

Acknowledgments

Edna Soraya Rawlings is grateful for partial support by the Center of Advanced Decision-making at Carnegie Mellon and CONACyT, Mexico. We would like to thank Jaffer H. Ghouse for his insightful advice on the initial stages of this work. This effort is part of the U.S. Department of Energy's Institute for the Design of Advanced Energy Systems (IDAES) supported by the Office of Fossil Energy's Crosscutting Research Program.

Abbreviations

CDC Continuous Distillation Column

DWC Dividing Wall Column

GDP General Disjunctive Programming

KC Kaibel Column

MINLP Mixed Integer Nonlinear Programming

n_e Dividing Wall Ending Tray

n_s Dividing Wall Starting Tray

NLP Nonlinear Programming

TAC Total Annual Cost

Nomenclature

2 Superindex representing the feed section in Kaibel column

3 Superindex representing the product section in Kaibel column

B Bottoms in mol/s

bu Boilup rate

C Set of components

C_C Cost of cold utility in \$/kWh

C_H Cost of heat utility in \$/kWh

C_{HE} Cost of heat exchangers in \$

C_{int} Cost of distillation column internals in \$

C_{shell} Cost of distillation column shell in \$

D Distillate in mol/s

d_L^w Liquid distributor for the dividing wall

d_V^w Vapor distributor for the dividing wall

γ Activity Coefficient

H Vapor enthalpy in J/mol

h Liquid enthalpy in J/mol

I_R Interest rate

J Total set of trays for the Kaibel column

J_1 Set of trays for the bottom section of the column for the GDP formulation

J_2 Set of trays for the feed section of the column for the GDP formulation

J_3 Set of trays for the product section 3 of the column for the GDP formulation

J_4 Set of trays for the top section of the column for the GDP formulation

J_B Set of trays for the bottom section of the column for the MINLP formulation

J_C Set of candidate trays for the main sections in the Kaibel column

J_E Set of existent trays for the main sections in the Kaibel column

J_T Set of trays for the top section of the column for the MINLP formulation

J_W Set of trays for the dividing walll sections of the column for the MINLP formulation

K Vapor-liquid equilibrium constant

L Liquid flowrate in mol/s

n_C Number of components

n_F Side feed tray

n_P Number of potential trays for the GDP formulation

n_T Number of trays

n_{R_1} Side tray for product outlet 1

n_{R_2} Side tray for product outlet 2

P^{sat} Vapor pressure in bar

P_L Plant life in years

Q_{con} Condenser heat duty in J/s

Q_{reb} Reboiler heat duty in J/s

S Set of main sections in the Kaibel column

V Vapor flowrate in mol/s

w Superindex representing the dividing wall sections

W Dividing wall sections 2 and 3

x Liquid composition in mol/mol

y Vapor composition in mol/mol

References

Barttfeld, M., Aguirre, P. A., and Grossmann, I. E. (2003). Alternative representations and formulations for the economic optimization of multicomponent distillation columns. *Computers and Chemical Engineering*, 27:363–383.

Barttfeld, M., Aguirre, P. A., and Grossmann, I. E. (2005). Optimal synthesis of complex distillation columns using rigorous models. *Computers and Chemical Engineering*, 29:1203–1215.

Caballero, J. A., Milan-Yañez, D., and Grossmann, I. E. (2005). Rigorous design of distillation columns: Integration of disjunctive programming and process simulators. *Ind. Eng. Chem. Res.*, 44:6760–6775.

Chen, Q., Johnson, E. S., Siirola, J. D., and Grossmann, I. E. (2018). Pyomo.gdp: Disjunctive models in python. *Computer Aided Chemical Engineering*, 44.

Dejanović, I., Matijaševic, L., and Olujić, Ž. (2010). Dividing wall column- A breakthrough towards sustainable distilling. *Chem. Eng. Process. Process Intensification*, 49:559–580.

Ghouse, J. H., Chen, Q., Zamarripa, M. A., Lee, A., Burgard, A. P., Grossmann, I. E., and Miller, D. C. (2018). A comparative study between GDP and NLP formulation for conceptual design of distillation columns. *Computer Aided Chemical Engineering*, 44:865–870.

Gomez-Castro, F. I., Segovia-Hernandez, J. G., Hernandez, S., and C. Gutierrez-Antonio, A. B.-R. (2008). Dividing wall distillation columns: Optimization and control properties. *Chem. Eng. Technol.*, 31:1246–1260.

Grossmann, I., Bonami, P., Biegler, L., Conn, A., Cornuejols, G., Laird, C., Lee, J., Lodi, A., Margot, F., Sawaya, N., and Wachter, A. (2005). *An Algorithmic Framework for Convex Mixed Integer Nonlinear Programs*. Elsevier.

Hart, W. E., Laird, C. D., Watson, J.-P., Woodruff, D. L., Hackebeil, G. A., Nicholson, B. L., and Siirola, J. D. (2017). *Pyomo–optimization modeling in python*, volume 67. Springer Science & Business Media, Second edition.

Hart, W. E., Watson, J.-P., and Woodruff, D. L. (2011). Pyomo: modeling and solving mathematical programs in python. *Mathematical Programming Computation*, 3(3):219–260.

Jackson, J. R. and Grossmann, I. E. (2001). A disjunctive programming approach for the optimal design of reactive distillation columns. *Computers and Chemical Engineering*, 25:1661–1673.

Kaibel, G. (1987). Distillation columns with vertical partitions. *Chemical Engineering Technology*, 10:92–98.

Kiss, A. A. and Baldea, C. S. (2011). A control perspective on process intensification in dividing wall columns. *Process Intensification*, 50:281–292.

Kiss, A. A., Landaeta, S. J. F., and Ferreira, C. A. I. (2012). Towards energy efficient distillation technologies - Making the right choice. *Energy*, 47:531–542.

Ling, H. and Luyben, W. L. (2010). Temperature control of the BTX divided-wall column. *Ind. Eng. Chem. Res.*, 49:189–203.

Lopez-Saucedo, E. S., Chen, Q., Grossmann, I. E., and Caballero, J. A. (2018). Kaibel column: Modeling and optimization. *Computer Aided Chemical Engineering*, 44:1183–1188.

Peters, M., Timmerhaus, K., and West, R. (2003). *Plant Design and Economics for Chemical Engineers*. McGraw-Hill Chemical Engineering Series 5th Edition.

Petlyuk, F. B., Platonov, V. M., and Slavinskii, D. M. (1965). Thermodynamically optimal method for separating multicomponent mixtures. *Int. Chemical Engineering*, pages 555–561.

Qian, X., Jia, S., Skogestad, S., and Yuan, X. (2016). Control structure selection for four-product Kaibel column. *Chemical Engineering and Processing*, 93:372–381.

Tututi-Avila, S., Dominguez-Diaz, L. A., Medina-Herrera, N., Jimenez-Gutierrez, A., and Hahn, J. (2017). Dividing-wall columns: Design and control of a Kaibel and a Satellite distillation column for a BTX separation. *Chemical Engineering and Processing*, 114:1–15.

U.S. Department of Energy (2001). Distillation Column Modeling Tools. `https://www1.eere.energy.gov/manufacturing/resources/chemicals/pdfs/distillation.pdf`. [Online; accessed October 10th, 2018].

Viswanathan, J. and Grossmann, I. E. (1990). A combined penalty function and outer approximation method for MINLP optimization. *Computers and Chemical Engineering*, 14:769–782.

Wachter, A. and Biegler, L. T. (2006). On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Mathematical Programming*, 106:25–57.

Yeomans, H. and Grossmann, I. E. (2000). Disjunctive programming models for the optimal design of distillation columns and separation sequences. *Ind. Eng. Chem. Res.*, 39:1637–1648.

Yildirim, O., Kiss, A. A., and Kenig, E. Y. (2011). Dividing wall columns in chemical process industry: A review on current activities. *Sep. Purif. Technol.*, 80:403–417.