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Set Trimming approach for the globally optimal design of sieve trays in separation columns

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Abstract

In this article, we use Set Trimming to obtain the globally optimal design of distillation column trays, that is, the column diameter and the geometrical design of the trays (weir, downcomer, etc.) that minimize mass or cost. We assume that the operating conditions (vapor and liquid flow rates, compositions, temperatures) are given. The design task is, to this day, presented in textbooks as a trial and verification procedure. We show that Set Trimming guarantees global optimality and is amenable to exploring alternative global optima. Compared with the employment of a mixed-integer nonlinear programming (MINLP) approach using commercial global optimizers, we show that Set Trimming is a more robust option with competitive computational times for individual design problems. It also exhibits a significant reduction in computational effort when alternative optimal solutions are sought.

KEYWORDS
design, distillation, optimization, Set Trimming, tray

1 | INTRODUCTION

The design of column trays in separation columns has been traditionally handled using trial-and-verification procedures through step-by-step procedures.[1–8] Some of these procedures are based on bold assumptions and heuristics that facilitate obtaining viable answers, with the intended effect of keep changing the trial geometries until one is viable. For example, the area of the downcomer is assumed to be 10% of the total area right after the diameter is selected based on a flooding velocity.[8]

The utilization of optimization techniques for the design of column trays was addressed by a few works. Ogboja and Kuye[9] used the Complex Method to solve a sieve tray optimization. They obtained the optimal tray design by maximizing tray efficiency according to geometrical and phenomenological constraints. The problem formulation was restricted to optimizing only one plate and not the total set of column trays. Lahiri[10,11] presented a method to obtain the optimal tray design based on the minimization of the total annualized cost, showing better results when compared with a commercial simulator. More recently, Souza et al.[12] presented a mixed-integer nonlinear mathematical model (MINLM) solved using a global optimizer for the design of column trays, based on the equations presented in Towler and Sinnot.[8]

As shown by Souza et al.,[12] the solution to the tray design-optimization problem using mathematical programming can attain better results than the traditional trial and verification approach. However, further numerical tests indicate that the global solution of the tray design problem using mathematical programming may be difficult sometimes. Aiming at providing a fast and reliable optimization tool for the solution of the optimal tray design problem, we present in this work the application of Set Trimming.[13] According to the results presented in this article, the proposed technique for solving the tray design problem is more robust than mathematical programming using global solvers, presenting competitive computational times.

Another important aspect of the proposed technique is the solution based on optimal sets, instead of optimal points. Conventional optimization techniques identify a single optimal solution. However, Set Trimming can identify all of the optimal solutions with the lowest value of the objective function (if there is more than one). Therefore, the user can choose one of these solutions considering other additional criteria that were not originally contemplated in the problem formulation. The identification of this set using conventional optimization techniques demands a recursive solution to the optimization problem, but Set Trimming can do it in a single run. We discuss more details about Set Trimming later in the article.

This article is organized as follows: Section 2 presents the geometric variables that are employed in the design problem, Section 3 presents the problem constraints, Section 4 presents different objective functions employed for the formulation of the design optimization problem, Section 5 presents the Set Trimming technique, and Section 6 illustrates the performance of the proposed formulation and compares it with mathematical programming. The conclusions are finally presented in Section 7.

2 | SIEVE TRAY GEOMETRY

The proposed optimization procedure is applied here for the design of sieve trays (the same optimization technique can be also employed for bubble cap or valve trays). A sieve tray is composed of the active and downcomer areas, with some calming zones. There are several types of configurations that use multiple passes (mostly for large diameters) and others, as well as different downcomer geometries (segmental, circular, etc.). Figure 1 shows the simplest configuration (one pass and segmental downcomer), which is the one we use in this article and our previous one.[12] Summarizing the detailed description given in the aforementioned article, we cite the components: active area (*Aa*), downcomers areas (*Adc*), hole area (*Ah*), calming zones (wcz_{in} and wcz_{out}), and unperforated strips (*wus*).

Figure 2 shows a side view of the tray highlighting another set of model variables: tray spacing (*lt*), weir height (*hw*), height of the liquid crest over the weir (*how*), clearance height under the downcomer (*hap*), the difference between weir and clearance height under the downcomer (*hdwap*), and the height of the downcomer backup (*hb*). The independent geometric variables we use are introduced in Table 1. The optimization problem consists of the determination of the values of these variables associated with the optimal value of one of the objective functions described in Section 4. These variables are discrete in practice, namely *dh*, *tt* and *lt*, because are standardized, while many other variables, namely *Dc*, *hdwap*, *hw*, *lw* and *lp* are usually considered continuous, but fabrication forces the use of discrete values. The tray mathematical model allows the determination of the values of the other model variables based on a given set of values of this set of independent variables.

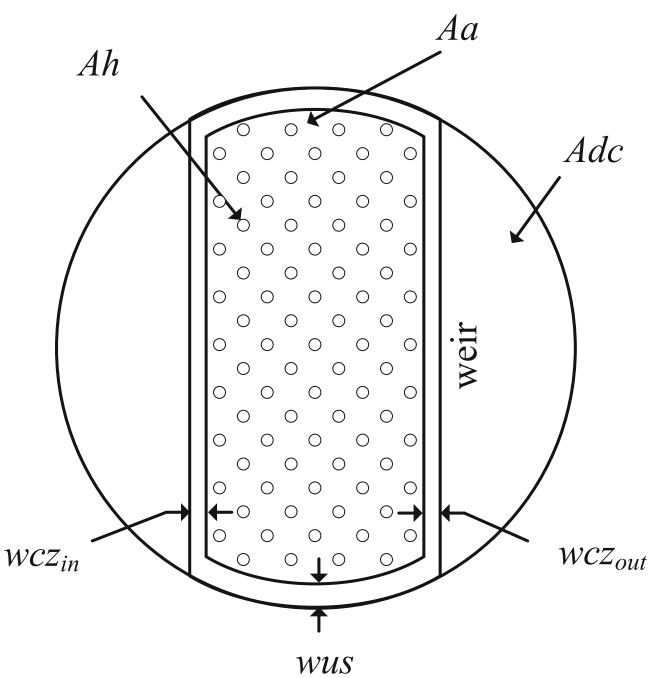

FIGURE 1 Sieve tray top view

Figure 3 depicts the downcomer area, which is obtained as the difference between the circular sector area (*Asector*) and the triangle area (*Atriangle*). The following equations show the geometrical relations among the several tray dimensions. Details of their development and source are given by Souza et al.[12]

The central angle of the circle that spans the weir is given by:

$$\theta = 2\arcsin\left(\frac{lw}{Dc}\right). \quad (1)$$

The area of the sector defined by the weir angle is:

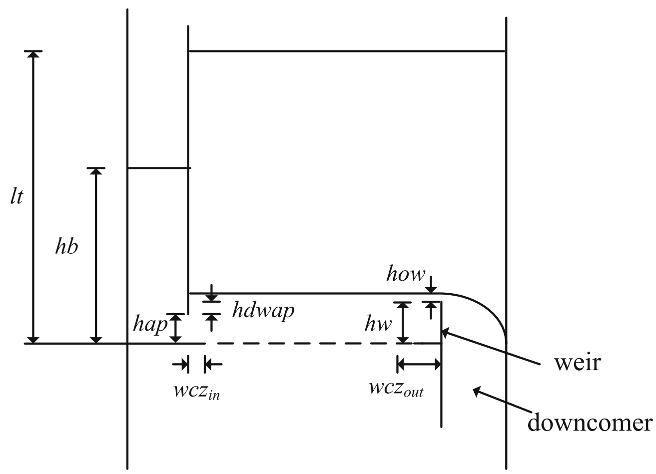

FIGURE 2 Tray side view

TABLE 1 Independent geometric variables

Variable	Definition	Unit
Dc	Column diameter	m
dh	Hole diameter	m
hdwap	Difference between weir and gap height	m
hw	Weir height	m
lt	Tray spacing	m
lw	Weir length	m
lp	Hole pitch	m
tt	Tray thickness	m
lay	Hole layout (triangle and squared)	–

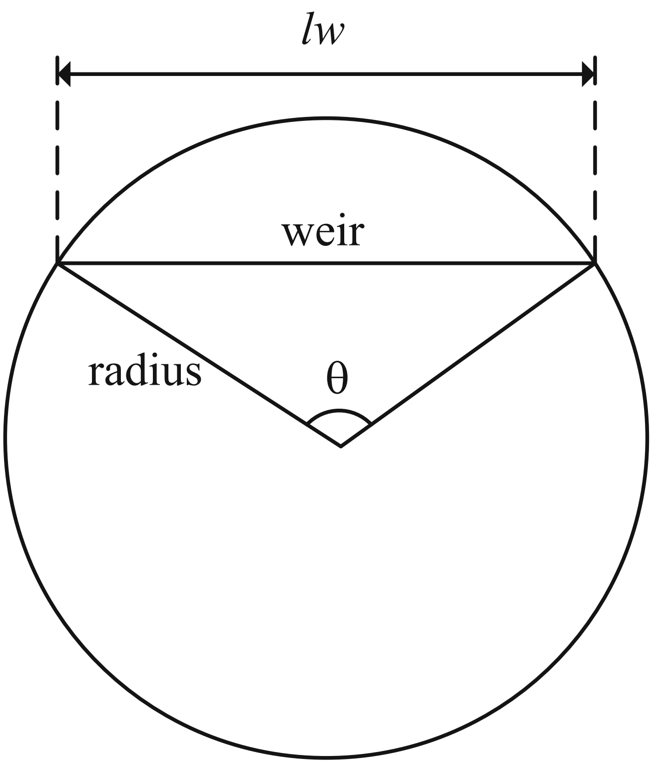

FIGURE 3 Tray downcomer area

$$Asector = \frac{Dc^2\theta}{8} \quad (2)$$

and the area of the triangle defined by the column radius and the weir length is:

$$Atriangle = \frac{lw}{2}\sqrt{\left(\frac{Dc}{2}\right)^2 - \left(\frac{lw}{2}\right)^2}. \quad (3)$$

The total column cross-sectional area (Ac), the cross-sectional area of the downcomer (Adc), and the net area available for vapor–liquid interaction (An) are given by:

$$Ac = \frac{\pi Dc^2}{4}, \quad (4)$$

$$Adc = Asector - Atriangle, \quad (5)$$

$$An = Ac - Adc. \quad (6)$$

Additional geometric relations involving the calming zones and unperforated strip areas are shown below, associated with the representation in Figure 4.

The calming zone area (Acz) is the area of two trapezoids, as illustrated in Figure 4, and it is given by:

$$Acz = \frac{(lcz_{in} + lw)}{2}\widehat{wcz}_{in} + \frac{(lcz_{out} + lw)}{2}\widehat{wcz}_{out}. \quad (7)$$

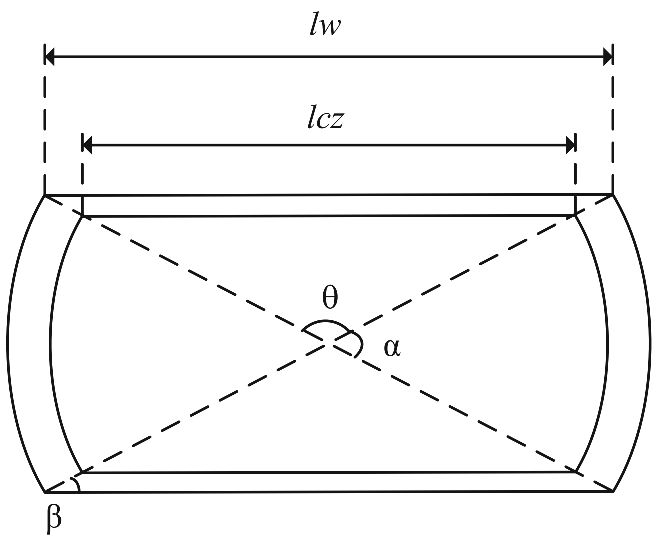

FIGURE 4 Calming zones and unperforated strip areas

The length of the calming zone (lcz) is given by:

$$lcz_{in} = lw - 2\left(\frac{\widehat{wcz}_{in}}{\tan\beta}\right), \quad (8)$$

$$lcz_{out} = lw - 2\left(\frac{\widehat{wcz}_{out}}{\tan\beta}\right), \quad (9)$$

where β is the calming zone angle:

$$\beta = \frac{\pi - \theta}{2}. \quad (10)$$

The width of the inlet and outlet calming zone has been suggested to be between 2 and 5 in.[2,8,14,15] Then, we consider $\widehat{wcz}_{in}$ and $\widehat{wcz}_{out}$ equal to 0.050 m (2 in.).

As a consequence, the unperforated strip area (Aus) is determined using the angle of the active area (α) and the width of the unperforated strip (wus).[8]

$$Aus = wus\,\alpha(Dc - wus), \quad (11)$$

$$\alpha = \pi - \theta. \quad (12)$$

The width of the unperforated strip varies according to diameter[15]:

$$wus = \begin{cases} 0.0381, & Dc \le 0.7620 \\ 0.0508, & 0.7620 < Dc \le 1.6764 \\ 0.0635, & 1.6764 < Dc \le 3.8100 \\ 0.0762, & 3.8100 < Dc \le 5.9436 \\ 0.0889, & 5.9436 < Dc \le 7.4676 \\ 0.1143, & Dc > 7.4676 \end{cases}. \quad (13)$$

The active area is the column cross-sectional area less the downcomer area, the unperforated strip area, and the calming zone areas:

$$Aa = Ac - 2\,Adc - Aus - Acz. \tag{14}$$

The hole area (Ah) can be determined as follows[16]:

$$Ah = k\left(\frac{dh}{lp}\right)^2 Aa, \tag{15}$$

where k is 0.785 or 0.905 from square or triangular hole layout, respectively.

3 | OPTIMIZATION CONSTRAINTS

The set of constraints involves geometric and operational constraints.

3.1 | Geometric constraints

The weir length must be limited to the column diameter:

$$lw \leq Dc. \tag{16}$$

The hole pitch must be equal to or greater than twice the hole diameter[8]:

$$lp \geq 2\,dh. \tag{17}$$

The thickness must be limited by the hole diameter[7]:

$$\frac{dh}{tt} \geq 1. \tag{18}$$

The ratio of the hole area to the active area is bounded:

$$0.06 \leq \frac{Ah}{Aa} \leq 0.16. \tag{19}$$

3.2 | Operational constraints

The operational constraints are the limits of flooding, entrainment, weeping, downcomer backup, and residence time in the downcomer of the sieve tray design. Because the flow rates and physical properties of the vapor and liquid stream vary along the column, these constraints must be applied for each tray, identified by the index sNt. These constraints are also reproduced below from Souza et al.[12] without further discussion.

- Flooding:

$$un_{sNt} \leq 0.85\,uflood_{sNt}\,\forall sNt, \tag{21}$$

$$un_{sNt} = \frac{\widehat{Vw}_{sNt}}{\widehat{\rho v}_{sNt}\,An}\forall sNt, \tag{22}$$

$$uflood_{sNt} = K1\,Csb_{sNt}\sqrt{\frac{\widehat{\rho l}_{sNt} - \widehat{\rho v}_{sNt}}{\widehat{\rho v}_{sNt}}}\left(\frac{\widehat{\sigma}_{sNt}}{0.02}\right)^{0.2}\forall sNt, \tag{23}$$

$$\widehat{Flv}_{sNt} = \frac{\widehat{Lw}_{sNt}}{\widehat{Vw}_{sNt}}\sqrt{\frac{\widehat{\rho v}_{sNt}}{\widehat{\rho l}_{sNt}}}\forall sNt, \tag{24}$$

$$K1 = \begin{cases} 0.8, & 0.06 \leq \dfrac{Ah}{Aa} \leq 0.08 \\ 0.9, & 0.08 \leq \dfrac{Ah}{Aa} \leq 0.10, \\ 1.0, & 0.10 \leq \dfrac{Ah}{Aa} \leq 0.16 \end{cases} \tag{25}$$

$$\begin{aligned} Csb_{sNt} = {} & 0.0129 + 0.1674\,lt + 0.0063\widehat{Flv}_{sNt} - 0.2686\,lt\,\widehat{Flv}_{sNt} \\ & - 0.008\widehat{Flv}_{sNt}^{\,2} + 0.01448\,lt\,\widehat{Flv}_{sNt}^{\,2}\,\forall sNt. \end{aligned} \tag{26}$$

- Entrainment

$$\psi_{sNt} \leq 0.1\,\forall sNt \tag{27}$$

$$\psi_{sNt} = \left\{ exp\left[\begin{array}{c} -7.9196 + 1.0891 Fflood_{sNt} \\ -(0.0705 + 2.1916 Fflood_{sNt})\ln\hat{Flv}_{sNt} \\ +\left(0.046 - 0.605 Fflood_{sNt} + 1.2669 Fflood_{sNt}^{\,2} - 0.9563 Fflood_{sNt}^{\,3}\right)\left(\ln\hat{Flv}_{sNt}\right)^2 \end{array} \right] \right\}\forall sNt, \tag{28}$$

Finally, to use the Fair flooding correlation, the following constraint holds[17]:

$$hw \leq 0.15\,lt. \tag{20}$$

Except for Equations (16) and (17), which are logical constraints, all the rest are heuristics.

$$Fflood_{sNt} = \frac{un_{sNt}}{uflood_{sNt}}\forall sNt. \tag{29}$$

- Weeping:

$$uh_{sNt} \geq uhmin_{sNt}\,\forall sNt, \tag{30}$$

$$uh = \frac{\widehat{Vw}_{sNt}}{\widehat{\rho v}_{sNt}\,Ah}\forall sNt, \tag{31}$$

$$uhmin_{sNt} = \frac{K2_{sNt} - 0.9\left(25.4 - 10^3 dh\right)}{\left(\widehat{\rho v}_{sNt}\right)^{\frac{1}{2}}} \forall sNt, \quad (32)$$

$$K2_{sNt} = 23.48 - 1.66 \ln\left[10^3 (hw + how_{sNt})\right] \forall sNt, \quad (33)$$

$$how_{sNt} = 750 \cdot 10^{-3}\left[\frac{\widehat{Lw}_{sNt}}{\widehat{\rho l}_{sNt}\, lw}\right]^{2/3} \forall sNt. \quad (34)$$

- Downcomer backup

$$hb_{sNt} \le \frac{1}{2}(lt + hw) \forall sNt, \quad (35)$$

$$hb_{sNt} = hw + how_{sNt} + ht_{sNt} + hdc_{sNt} \forall sNt, \quad (36)$$

$$ht_{sNt} = hw + how_{sNt} + hd_{sNt} + \widehat{hr}_{sNt} \forall sNt, \quad (37)$$

$$\widehat{hr}_{sNt} = \frac{12.5}{\widehat{\rho l}_{sNt}} \forall sNt, \quad (38)$$

$$hd_{sNt} = 51 \cdot 10^{-3}\left(\frac{uh_{sNt}}{Co}\right)^2 \frac{\widehat{\rho v}_{sNt}}{\widehat{\rho l}_{sNt}} \forall sNt, \quad (39)$$

$$Co = 0.6323 - 0.0255\frac{tt}{dh} + 0.1495\left(\frac{tt}{dh}\right)^2 + 0.777\frac{Ah}{Aa}, \quad (40)$$

$$hdc_{sNt} = 166 \cdot 10^{-3}\left(\frac{\widehat{Lw}_{sNt}}{\widehat{\rho l}_{sNt}\, Aap}\right) \forall sNt, \quad (41)$$

$$Aap = hap\, lw, \quad (42)$$

$$hap = hw - hdwap. \quad (43)$$

- Residence time:

$$time_{sNt} \ge 3\,s \forall sNt, \quad (44)$$

$$time_{sNt} = \frac{Adc\, hb_{sNt}\, \widehat{\rho l}_{sNt}}{\widehat{Lw}_{sNt}} \forall sNt. \quad (45)$$

4 | OBJECTIVE FUNCTION

The optimization proposal consists in minimizing the costs associated with the sieve tray design of a distillation column. Two alternative objective functions are explored: a capital cost equation and an expression of the mass of the distillation column.

The cost equation is given by (assuming a carbon steel column)[8]:

$$Min\, Ctotal = \left(130 + 440 Dc^{1.8}\right)\widehat{Nt} + 11{,}600 + 34\, Wshell^{0.85}, \quad (46)$$

where $\widehat{Nt}$ is the number of trays and $Wshell$ is the mass of the column shell. The equation is validated from $0.5 < Dc < 5.0$ m and $160 < Wshell < 250{,}000$ kg. The mass of the column shell is given by:

$$Wshell = \pi\, \widehat{\rho shell}\, Dc\, Hc\, twall, \quad (47)$$

where $\widehat{\rho shell}$ is the density of the shell material, $twall$ is the column wall thickness and Hc is the height of the column between tangent lines, given by:

$$Hc = \widehat{Nt}\, lt. \quad (48)$$

Another alternative objective function consists in minimizing the mass of the distillation column and its trays ($Wtotal$):

$$Min\, Wtotal = Wcolumn + Wt\, \widehat{Nt}. \quad (49)$$

The mass of the column is given by[8]:

$$Wcolumn = \widehat{Cw}\, \pi\, \widehat{\rho shell}\, Dm (Hc + 0.8 Dm) twall, \quad (50)$$

where $\widehat{Cw}$ is a factor responsible by the mass of nozzles, manways, internal supports, and so forth, to distillation columns is 1.15 and Dm is the mean diameter of the column, given by:

$$Dm = Dc + twall. \quad (51)$$

The mass of the tray is determined by the volume of the tray (Vt) and the volume of the weir together with the downcomer ($Vwdc$).

$$Wt = (Vt + Vwdc)\widehat{\rho t}, \quad (52)$$

where $\widehat{\rho t}$ is the specific mass of tray material. The volume of the tray (Vt) is given by the area of the column minus the areas of the downcomer and holes, and the volume of the combination weir/downcomer ($Vwdc$) is given by a rectangular plate:

$$Vt = (Ac - Adc - Ah) tt, \quad (53)$$

$$Vwdc = [hw + tt + Hdc]\, tt\, lw, \quad (54)$$

where Hdc is the height of downcomer:

$$Hdc = lt - hap = lt - (hw - hdwap). \quad (55)$$

5 | SET TRIMMING

The Set Trimming technique was initially proposed by Gut and Pinto[18] for the specific case of the design of plate heat exchangers. Costa and Bagajewicz[13] generalized it conceptually to apply to any optimization problem with discrete independent variables. The same technique was successfully applied by Lemos et al.[19] and Nahes et al.[20] to the design optimization of shell and tube heat exchangers and plate heat exchangers, respectively.

The Set Trimming technique is applied to problems with a combinatorial representation of the search space, where each candidate solution corresponds to a set of discrete values of the decision variables. The technique consists of applying the inequality constraints sequentially to the set of candidates so that after testing each constraint, the number of candidates decreases. Thus, in the end, if all constraints are applied, only feasible candidates remain, that is, the candidates that respected all the constraints of the model. Consequently, after Set Trimming, the global optimum can be obtained through a simple sorting procedure applied to the objective function of the feasible candidates. This technique is a global optimization technique because only the infeasible candidates are eliminated and, in the end, there is a selection, to obtain the best alternative among feasible candidates.[13]

The steps of each trim of Set Trimming method, using the model of the sieve tray design are shown below, according to the representation depicted in Figure 5. In these steps, each set is defined as a subset of the previous one, thus eliminating the infeasible candidates from each step. The initial candidate set is the set of all combinations of the independent geometric variables of the problem (Table 1).

The Set Trimming starts with the geometrical constraints, that is, using the inequalities Equations (16)–(20). This set of constraints trims the majority of candidates for which some of the operational limits do not even make sense. The application of all the other operational inequalities follows. The order of the trims was selected through an analysis of the computational efficiency of the elimination of candidates provided by each constraint (see Section 6). After Set Trimming, the optimal solution is identified through a simple sorting procedure of the values of the objective function of the feasible candidates.

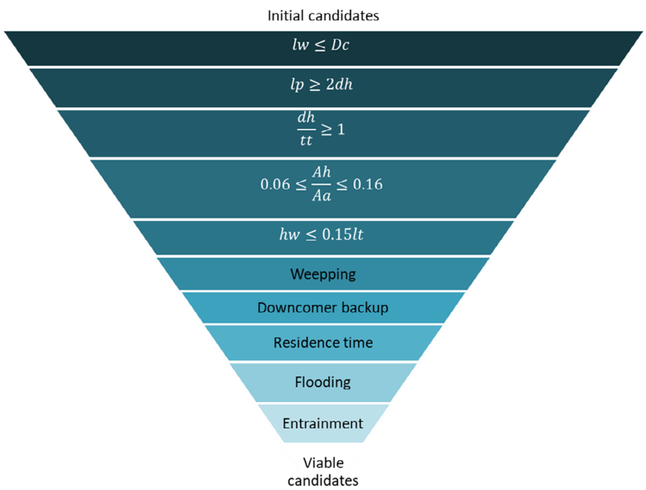

FIGURE 5 Set Trimming structure

6 | POWER ANALYSIS

The order of the constraints in the Set Trimming is very important for its computational performance. Because the time used to trim a set depends on its size, one wants to identify what are the constraints that trim the largest amount of candidates. However, the time to evaluate each constraint also matters. Therefore, both need to be taken into account.

Aiming at identifying the effectiveness of the trim action associated with each constraint, we use the following procedure. Using the first set of candidates obtained after geometric Set Trimming as a starting point, we apply each constraint separately. Thus, based on the number of candidates eliminated and the computational time spent on each constraint, it is possible to determine the fraction of candidates eliminated and the number of candidates eliminated per second by each trim action. The power of each constraint is in eliminating more candidates in less time.

After that, the appropriate ordering of the constraints is determined by picking the constraints in descending order of power (number of candidates eliminated/second). Therefore the trimmings of the constraints that are slower and eliminate fewer candidates will be applied later, which will provide a reduction in the computational time. While this ordering is not guaranteed to render the smallest computational time in all cases (it still depends on the particular problem), it is a step in the right direction.

7 | RESULTS

We use an example taken from Towler and Sinnott,[8] where acetone is recovered from a 10% mol of acetone aqueous waste. The top stream of the distillation column must contain 95% mol of acetone and the bottom stream must not contain more than 1% mol of acetone. The number of real stages is 15, considering a column efficiency of 60% and excluding the reboiler. The column material was carbon steel ($\widehat{\rho shell} = \widehat{\rho t} = 7900\ \mathrm{kg/m^3}$).

Table 2 presents the operational parameters of the nine ideal stages, with stage 8 as the feed tray. These were obtained by a

TABLE 2 Operational parameters of the investigated example

Parameter	1	2	3	4	5	6	7	8	9
$\widehat{Lw}$ (kg/s)	0.82	0.80	0.78	0.76	0.72	0.66	0.51	3.12	2.78
$\widehat{Vw}$ (kg/s)	1.50	1.48	1.46	1.43	1.40	1.34	1.18	1.02	0.68
$\widehat{\rho l}$ (kg/m^3)	753.76	754.64	755.64	756.92	758.84	762.57	776.27	873.01	900.73
$\widehat{\rho v}$ (kg/m^3)	2.10	2.09	2.07	2.04	2.01	1.95	1.78	1.61	1.02
$\widehat{\sigma}$ (N/m) $\times 10^3$	22.28	23.20	24.21	25.45	27.21	30.28	38.60	59.14	60.79

simulation in the Aspen Plus software using the property package UNIQ-RK, which employs the Redlich–Kwong equation of state[21] and the UNIQUAC activity coefficient model.[22] The reflux ratio is 1.24.

Table 3 presents the standard alternatives of the geometric variables. The column diameters vary between 0.6096 m (2 ft–24 in.) and 4.826 m (15.8 ft–190 in.), the lower limit is the diameter needed to avoid installation difficulties, and the upper limit is the largest diameter for which the cost equation is valid.[8] This set of diameters is selected in such a way that the differences between the diameter values increases as the diameter increases. Table 4 shows the values of the column shell thickness related to each column diameter alternative, according to Towler and Sinnott.[8] Further details of the selection of the possible values for the other design variables can be found in Souza et al.[12] All the computational results presented here were obtained using a computer with Intel Core i7 (8th Gen) processor with 8 Gb of RAM, using GAMS version 24.7.1 (it is important to mention that none of the GAMS solvers was used to implement the Set Trimming algorithm, only the manipulation resources of sets were employed).[23]

The result of the power analysis is shown in Table 5. The initial number of candidates where those constraints are applied corresponds to 738,900. We conclude that the weeping and residence time are the sets that quickly eliminate a large number of candidates, and for this reason, they should be applied first. Downcomer backup calculations are needed for the evaluation of the residence time so this precedence order is preserved. The sets of flooding and entrainment are the last conditions because they eliminate few candidates per unit time.

The computational time employed by Set Trimming using the sequence determined by the power analysis is shown in Table 6. Table 6 also shows the computational time of a different arbitrary sequence. We observe that this sequence is associated with a computational time that is almost double the one obtained using the sequence determined by the power analysis, which illustrates the importance of a proper ordering of the constraints in the Set Trimming procedure and the effectiveness of the power analysis to provide a good sequence. We remark that this choice is not universal. A study analyzing several different columns with different vapor and liquid traffic might reveal different sequences to be more efficient under specific flow rate traffic conditions.

The results of the application of the technique of Set Trimming with the objective function column cost (Equation 46) are shown in Table 7, where the number of candidates after the trim using each constraint is shown.

According to Table 7, the search space of the optimization problem is composed of 7,931,520 candidates. The Set Trimming procedure identifies only 18,097 (0.22%) feasible design alternatives. We observe that the operational constraints (Equations 21–45) are applied to a considerably lower number of candidates, which is a fundamental aspect of the computational efficiency of the Set Trimming procedure.

After the Set Trimming procedure, the optimal solution can be identified through the application of a simple sorting procedure. The results of the sorting procedure are presented in Table 8, which shows the number of feasible candidates identified by the Set Trimming and

TABLE 3 Candidate dimensions for the design variables

Variables	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Dc (m–in)	0.61	0.76	0.91	1.07	1.27	1.47	1.68	1.93	2.18	2.44	2.74	3.05	3.35	3.71	4.06	4.42	4.83
	24	30	36	42	50	58	66	76	86	96	108	120	132	146	160	174	190
dh (mm–in)	3.60	4.00	4.40	4.80	5.20	5.60	6.00	6.40									
	9/64	5/32	11/64	3/16	13/64	7/32	15/64	1/4									
hdwap (mm)	5.00	6.00	7.00	8.00	9.00	10.0											
hw (cm–in)	3.81	4.44	5.08	5.71	6.35	6.98	7.62	8.25	8.89								
	1 1/2	1 3/4	2	2 1/4	2 1/2	2 3/4	3	3 1/4	3 1/2								
lt (m–in)	0.15	0.23	0.31	0.47	0.62	0.91											
	6	9	12	18	24	36											
lw (m–in)	0.41	0.66	0.91	1.17	1.42	1.68	1.93	2.18	2.44	2.69	2.95	3.20	3.45	3.71	3.96		
	16	26	36	46	56	66	76	86	96	106	116	126	136	146	156		
lp (mm)	9.00	12.0	15.0	18.0	21.0	24.0											
tt (mm)	3.40																
lay	Square		Triangular														

TABLE 4 Shell thickness for each column diameter

Dc (m)	0.61	0.76	0.91	1.07	1.27	1.47	1.68	1.93	2.18	2.44	2.74	3.05	3.35	3.71	4.06	4.42	4.83
twall (mm)	5	5	5	7	7	7	7	7	9	9	10	12	12	12	12	12	12

TABLE 5 Power analysis of Set Trimming

Constraint	Candidates eliminated	Fraction of candidates eliminated	Computational time (s)	Candidates eliminated per second
Flooding	13,680	1.75%	49.77	274.86
Entrainment	13,716	1.75%	49.52	276.98
Weeping	739,032	94.28%	48.25	15,316.73
Downcomer backup	26,384	3.37%	63.08	418.26
Residence time	233,160	29.74%	59.52	3917.34

TABLE 6 Set Trimming computational time using two different sequences of constraints

Constraint order	Time (s)
Power analysis: Weeping/Downcomer backup/Residence time/Flooding/Entrainment	43.66
Arbitrary: Flooding/Entrainment/Weeping/Downcomer backup/Residence time	84.14

TABLE 7 Number of active candidates after the trim related to each constraint

Constraint	Number of active candidates
Starting set	7,931,520
Geometric 1—max *lw*	4,167,936
Geometric 2—min *lp*	3,560,112
Geometric 3—max *hw*	1,648,200
Geometric 4—min *Ah*/*Aa*	924,600
Geometric 5—max *Ah*/*Aa*	738,900
Weeping	44,868
Downcomer backup	27,286
Residence time	18,587
Flooding	18,301
Entrainment	18,097

TABLE 8 Candidates sharing the same optimal objective function values

	Objective function	
Sorting	Cost	Mass
Number of feasible candidates	18,097	18,097
Candidates with the minimum objective function	354	5
Candidates in the subset featuring minimum ΔP	6	1

the number of candidates sharing the lowest value of the objective function. Two alternative objective functions are considered: cost (Equation 46) and mass (Equation 49). The optimal values obtained for both objective functions, $ 28,915.69 and 1335.52 kg, respectively, are the same as the ones found by Souza et al.[12]

TABLE 9 Optimal design variables

	Objective function	
Variable	Cost	Mass
Dc (m)	0.9144	0.9144
dh (m)	0.0036	0.0036
hdwap (m)	0.005	0.005
hw (m)	0.0381	0.0381
lt (m)	0.4572	0.4572
lw (m)	0.6604	0.6604
lp (m)	0.009	0.009
lay	Triangular	Triangular
Cost ($)	28,915.69	28,915.69
Mass (kg)	1335.52	1335.52
ΔP (N/m^2)	6254.94	6254.94

Because there are multiple candidates with the same value of the objective function, it is possible to apply a second criterion to the optimal set. This feature of Set Trimming allows the user to analyze the final set of solutions with the lowest value of the objective function to consider other aspects of the problem. In our case, we use a second sorting to identify the subset of optimal candidates with the lowest pressure drop (ΔP):

$$\Delta P = \hat{g} \sum_{sNt} ht_{sNt} \hat{\rho} l_{sNt}, \tag{56}$$

where $\hat{g}$ is the gravity acceleration. According to Table 8, there are six candidates with the lowest pressure drop with optimal cost and a single candidate with the lowest pressure drop with minimal mass. In both cases, the smallest value of pressure drop is 6254.94 N/m^2 (0.907 psi), which is relatively low.

The optimal values of the design variables with the smallest pressure drop are presented in Table 9. Among the six candidates of optimal cost and smallest pressure drop, the *hdwap* is the only variable that changes among all candidates. We remark that this variable has no effect on pressure drop, which explains the multiplicity of results. The results correspond to the lowest height of the liquid in the downcomer backup.

The histogram in Figure 6 shows the distribution of column costs for the 18,097 feasible candidates identified by the Set Trimming technique. In this histogram, the minimum cost of $ 28,915.69, associated with only 354 candidates, corresponds to less than 2% of the total of feasible candidates. Among the objective function values of the feasible candidates, there are several alternatives with objective function values much higher than the optimum value, some up to 115% more expensive. These data indicate that just guaranteeing a

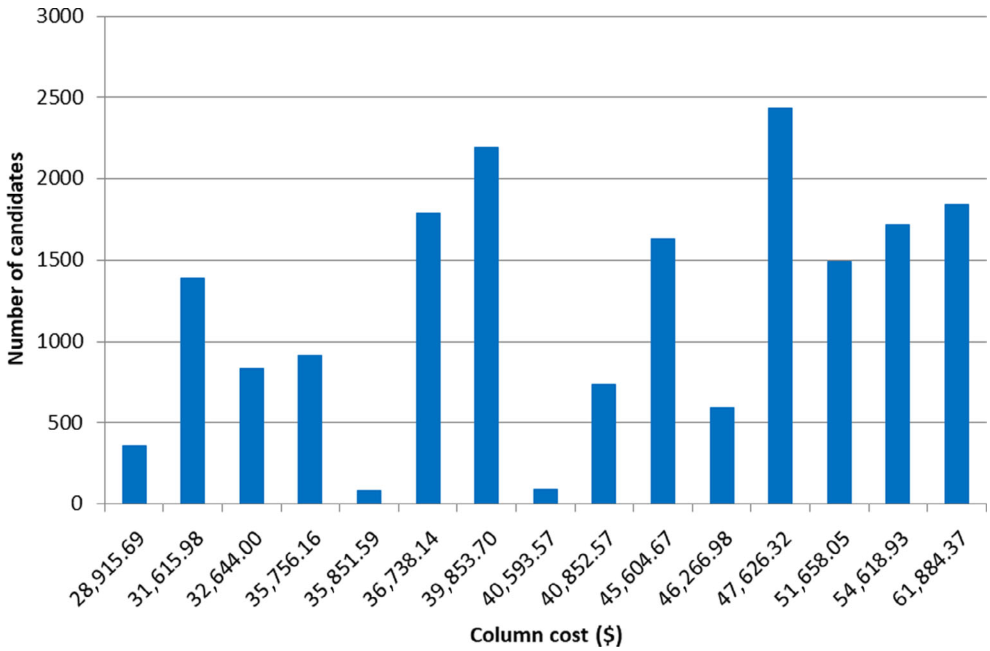

FIGURE 6 Histogram of the column cost of the feasible alternatives

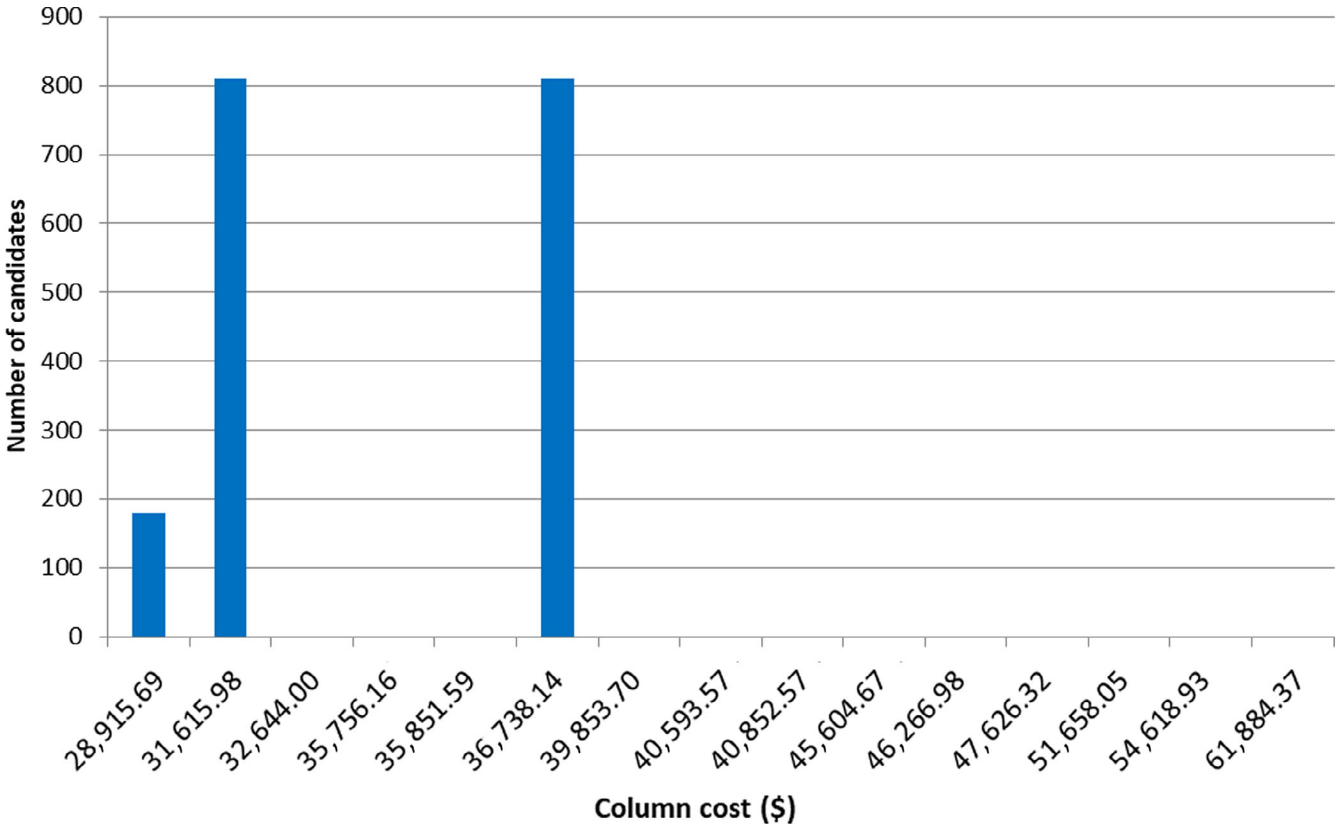

FIGURE 7 Histogram of the column cost, heuristic results

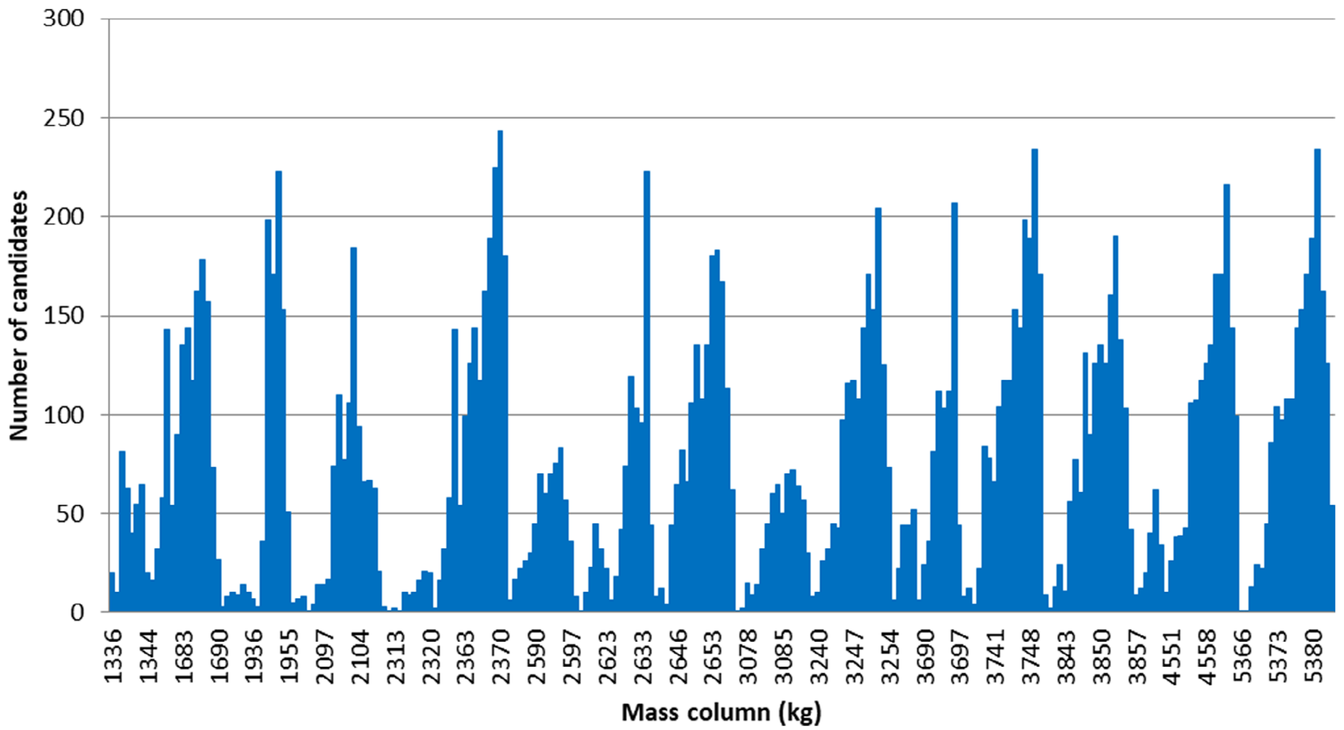

FIGURE 8 Histogram of the column mass of the feasible alternatives

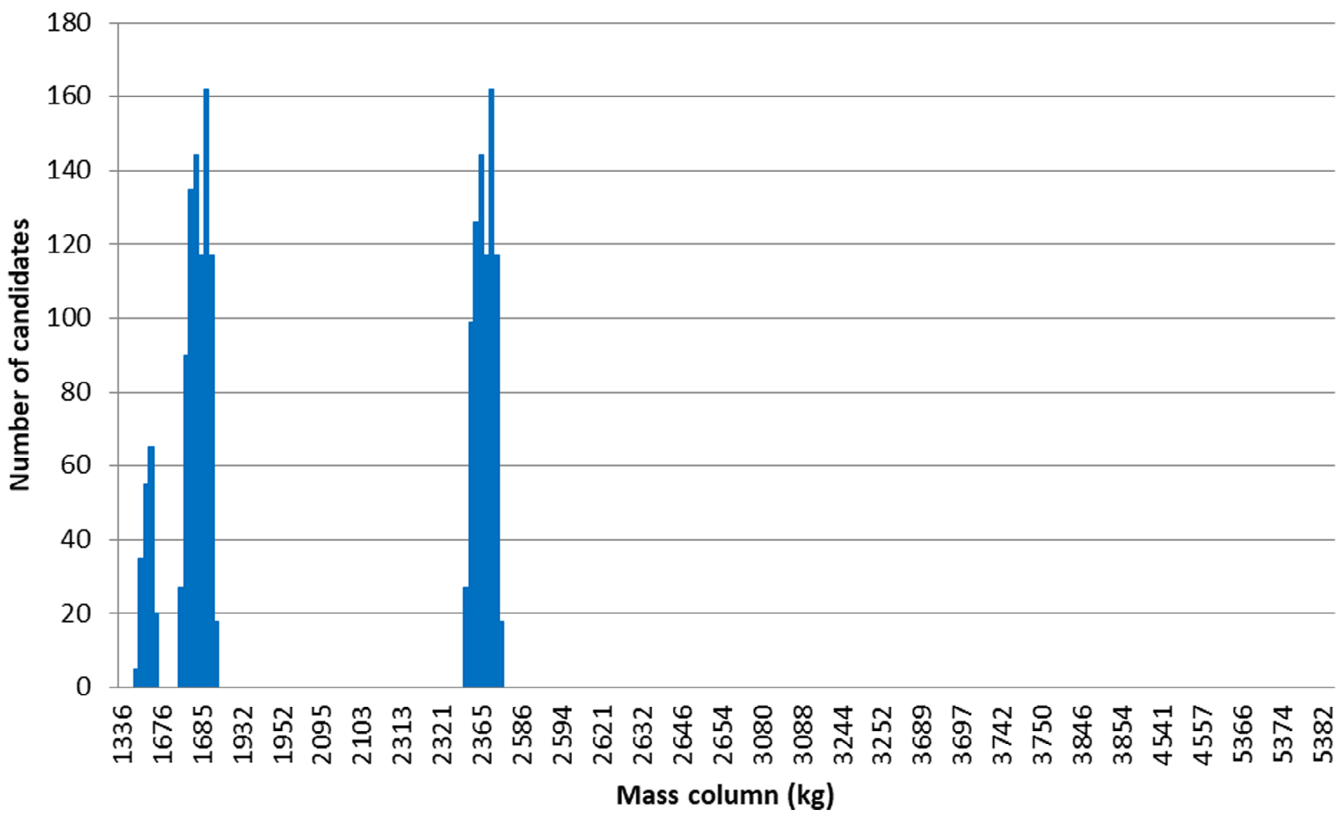

FIGURE 9 Histogram of the column mass, heuristic results

feasible solution as a result of the design can imply high costs, thus questioning the value of trial-and-verification procedures.

Design textbooks present heuristics that aim to guide the designer to a "good" solution. Towler and Sinnot[8] suggested the following values for the ratios *Adc*/*Ac* and *Ah*/*Aa*: 0.12 and 0.10, respectively. Therefore, one can identify which solution candidates present similar ratios of this type, within the bounds:

$$0.09 \leq \frac{Adc}{Ac} \leq 0.15, \tag{57}$$

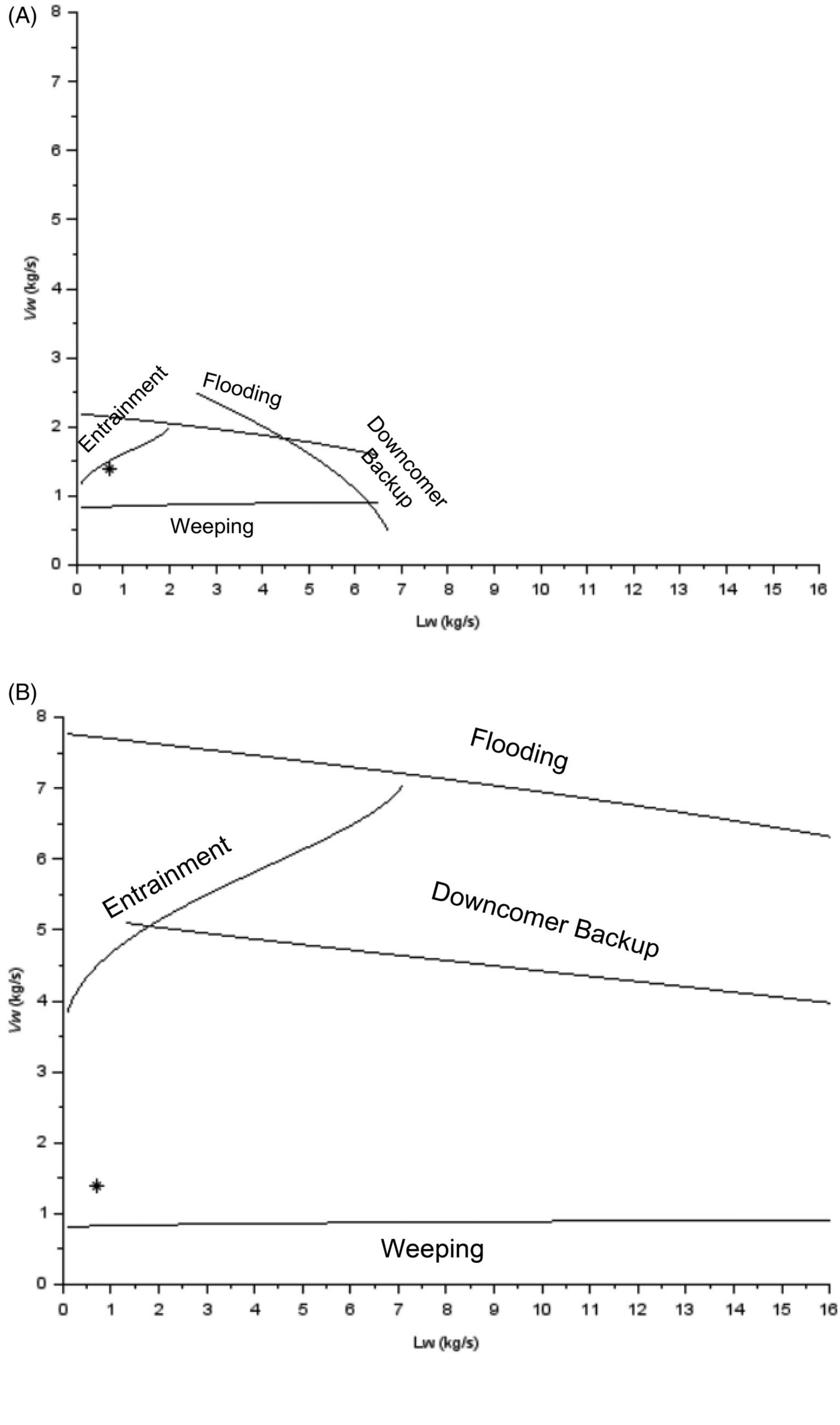

FIGURE 10 Sieve tray performance diagram. (A) Optimal tray: $Dc = 0.9144$ m, $dh = 0.0036$ m, $hdwap = 0.005$ m, $hw = 0.0381$ m, $lt = 0.4572$ m, $lw = 0.6604$ m, $lp = 0.009$ m, $lay =$ triangular. (B) Expensive tray: $Dc = 1.4732$ m, $dh = 0.0036$, $hdwap = 0.005$ m, $hw = 0.0381$ m, $lt = 0.9144$ m, $lw = 1.4224$ m, $lp = 0.009$ m, $lay =$ triangular

$$0.08 \le \frac{Ah}{Aa} \le 0.12. \quad (58)$$

The histogram of all feasible options, which comply with the heuristics conditions according to Equations (57)–(58), is given in Figure 7. We observe that the heuristics are useful to eliminate a large number of expensive candidates. However, the number of optimal candidates is still a small fraction of the set of candidates: the optimal candidates are only 10% of the total number of candidates that follows the heuristics, that is from the histogram, we conclude that there is only 10% chance that a designer that follows the heuristics picks a column of minimum cost. Likewise, there is a 45% chance that the designer can pick a solution with a 27% higher cost. We also note that among the set of columns of minimum cost, only 180 of the 354 feasible columns follow the guidelines. Incidentally, among the six columns with minimum pressure drop, all follow the heuristic condition of *Adc*/*Ac* and none follow the heuristic condition of *Ah*/*Aa*.

Figure 8 shows the histogram with the distribution of column mass for the 18,097 feasible candidates identified by the Set Trimming technique. We observe that 20 of 18,097 candidates (0.11%) present a mass of 1336 kg, close to the optimum shown in Table 9. Without an optimization tool, an inexperienced designer could find a feasible column up to 4 times heavier than the optimum. Roughly, the probability of this event is 10%.

The histogram based on mass, presented in Figure 9, shows all the feasible options which comply with the heuristics conditions. In this histogram, there is only 10% of the solutions that follow the heuristics close to the optimum (1340–1344 kg) and 45% of the heuristic-based solutions have a mass around 77% heavier than the optimum. Therefore, there is a considerable chance that a designer that follows the heuristics get a poor solution.

The sieve tray performance diagram is illustrated in Figure 10. This figure shows the operating point (vapor and liquid flow rates, for tray 5) and the area of the satisfactory operation, bounded by tray stability limits: entrainment, flooding, downcomer backup, and weeping. The operational point must be inside the area of satisfactory operation.

Figure 10A shows the results for the minimum cost solution ($ 28,915.69) and Figure 10B shows the results of a tray with a $ 61,884.37 cost. The satisfactory operating area depends on the geometric variables of the trays. For each different tray, the curves of the operating limits change, but the operating point remains the same. The comparison of Figure 10A,B indicates that the large cost of the latter is associated with oversizing. The expensive tray can be used for other operating points with different liquid and vapor flows, while the optimal tray, should only be used for operating points close to the ones in the example because it has a smaller operating area.

8 | COMPUTATIONAL COMPARISON WITH THE MINLP APPROACH

The computational performance of the proposed Set Trimming procedure for column tray design is compared with the mathematical programming of the Mixed-Integer Nonlinear Model (MINLM) described in Souza et al.,[12] using different solvers: Antigone 1.1 and Baron 16.3.4. All of the tests involving mathematical programming were conducted using default initial estimates and a stopping criterion of 0% gap between the upper and lower bounds.

To provide a clearer assessment of the comparison of the performance of Set Trimming and mathematical programming, the tests were conducted using 32 different optimization runs. The runs were based on the tray design problem presented above, for both objective functions, and associated with different sets of values of the liquid and vapor flow rates as well as different search spaces. The set of tested distillation column flow rates corresponds to the values reported in Table 2 multiplied by 0.5, 1.0, 2.0, and 3.0. The tested search spaces were generated through an increase of the number of possible values for the column diameters (the search space of the other variables was not modified), therefore, the corresponding tested sample was composed of 7,931,520 candidates, 9,331,200 candidates, 10,730,880 candidates, and 12,130,560 candidates. The details of each run are shown in the Supplementary Material, where the objective function and the computational time employed by each solution method are reported.

The analysis of the values of the optimal objective function of each run indicates that Set Trimming always finds the lowest cost solution. Despite the global nature of the solvers Antigone and Baron, the lowest-cost solution was not found in a considerable fraction of the test sample. Antigone solutions were trapped in a local optimum in 13 runs (41% of the sample). Baron did not converge in 5 runs (16% of the sample) and was trapped in a local optimum in 8 runs (25% of the sample).

Among the set of runs where the mathematical programming solver attained the lowest value of the objective function (19 Antigone and Baron runs), an analysis of the computational time indicates that Set Trimming was faster than Antigone in 8 runs (42% of this sample) and faster than Baron in 12 runs (63%).

Another comparison was done asking that mathematical programming finds other solutions with the same optimal cost, the same way as Set Trimming. To do this, we added in mathematical programming the following constraints that remove the previously found solution.

$$\sum_i \widehat{A}_{i,j} yx_i - \left(\widehat{B}_j - 1\right) \le 0, \quad (59)$$

$$\widehat{A}_{i,j} = \begin{cases} 1, & \text{if } yx_i = 1 \\ -1, & \text{if } yx_i = 0 \end{cases}, \quad (60)$$

$$\widehat{B}_j = \sum_i \widehat{A}_{i,j}, \forall \widehat{A}_{i,j} = 1, \quad (61)$$

where i is a set of binary variables, j is a set of constraints, $\widehat{A}_{i,j}$ and $\widehat{B}_j$ are parameters. Then, for each new solution, a new constraint is added to the set j. The variable x is related to the corresponding set of binary variables by:

$$x = \sum_i \widehat{px}_i yx_i, \quad (62)$$

$$\sum_i yx_i = 1. \tag{63}$$

After adding these equations to the mathematical programming formulations using a recursive algorithm, the solvers Antigone and Baron could identify only three least-cost solutions in 121 and 150 s, respectively. Thus, comparing Set Trimming and mathematical programming, Set Trimming obtained a set of 354 least-cost solutions in 43.66 s, while mathematical programming fails to obtain all and employs three times as much time to obtain only 3 of the 354 solutions.

A similar procedure was applied for the identification of the set of least-cost solutions with minimum pressure drops. In this case, the mathematical programming formulations were modified by substituting the objective function to use the minimization of the pressure drop and the insertion of an additional constraint of an upper bound on the cost, equivalent to the minimum cost already found. The minimization of pressure drop after minimizing the cost using the solver Antigone identified all six solutions in 108.44 s. The same procedure using Baron could not identify a solution. The Set Trimming obtained the six solutions in 43.66 s.

9 | CONCLUSIONS

This article presented a method to obtain a globally optimal design of distillation column trays, determining the independent geometrical variables of the tray. Two alternative objective functions were studied: minimization of column cost and mass. The method used is Set Trimming, to sequentially eliminate alternatives that do not follow the inequality constraints.

The analysis of the optimization results indicates that the results found for Set Trimming, after the sorting step, would unlikely be found by a designer guided by heuristic rules.

Another important aspect of the Set Trimming procedure is its capacity to identify all of the global optima of the problem. Therefore, the user can analyze the different optimal solutions, considering other aspects of the problem to choose the more adequate alternative. A similar result using mathematical programming demands a set of recursive runs, which is computationally expensive.

A comparison with two different global solvers (Antigone and Baron) indicates that Set Trimming is more robust than MINLP approaches. For a given sample of optimization problems, Set Trimming always attained the lowest value of the objective function, but mathematical programming approaches were trapped in a local optimum or did not converge in a considerable number of runs. The computational time of the Set Trimming runs was competitive when compared with the mathematical programming runs.

Therefore, because of its robustness and computational efficiency, the proposed procedure can be a useful tool for the design of distillation columns, especially in situations where its recursive use is needed, such as in design under uncertainty.

NOMENCLATURE

Aa	active area (m^2)
Aap	clearance area under the downcomer (m^2)
Ac	total column area (m^2)
Acz	calming zone area (m^2)
Adc	downcomer area (m^2)
Ah	hole area (m^2)
An	vapor flow area (m^2)
$Asector$	circular sector area (m^2)
$Atriangle$	triangle area (m^2)
Aus	unperforated strip area (m^2)
Co	orifice coefficient
Csb	Sounders–Brown coefficient (m/s)
$Ctotal$	total cost of column ($)
$\widehat{Cw}$	factor of cost equation (dimensionless)
Dc	column diameter (m)
dh	hole diameter (m)
Dm	mean diameter of column (m)
$Fflood$	percentage of flooding (%)
$\widehat{Flv}$	liquid–vapor flow factor (dimensionless)
$\widehat{g}$	gravity acceleration (m^2/s)
hap	height of the clearance under the downcomer (m)
hb	height of the downcomer backup
Hc	height of column, between tangent lines (m)
hd	dry tray drop (m)
hdc	pressure drop in the downcomer (m)
Hdc	height of downcomer (m)
$hdwap$	difference between weir and clearance height under the downcomer (m)
how	height of the liquid crest over the weir (m)
$\widehat{hr}$	residual pressure drop (m)
ht	total tray pressure drop (m)
hw	weir height (m)
$K1$	constant of Fair flooding correlation (dimensionless)
$K2$	constant of weeping correlation (dimensionless)
lay	hole layout
lcz_{in}	length of inlet calming zone (m)
lcz_{out}	length of outlet calming zone (m)
lp	hole pitch (m)
lt	tray spacing (m)
lw	weir length (m)
$\widehat{Lw}$	liquid mass flow rate (kg/s)
$\widehat{Nt}$	number of trays
$time$	residence time (s)
tt	tray thickness (m)
$twall$	column wall thickness (m)
$uflood$	flooding velocity (m/s)
uh	flow velocity throughout the tray holes (m/s)
$uhmin$	minimum vapor flow velocity (m/s)
un	vapor flow velocity (m/s)
Vt	volume of the tray (m^3)
$\widehat{Vw}$	vapor mass flow rate (kg/s)
$Vwdc$	volume of the combination weir/downcomer (m^3)

$\widehat{wcz}_{in}$ width of inlet calming zone (m)
$\widehat{wcz}_{out}$ width of outlet calming zone (m)
Wcolumn mass of the column shell and internals (kg)
Wshell mass of the column shell (kg)
Wt mass of the tray (kg)
Wtotal mass of the distillation column (kg)
wus width of unperforated strip (m)

GREEK SYMBOLS

α active area angle (rad)
β calming zone angle (rad)
ΔP pressure drop (N/m^2)
θ weir angle (rad)
ψ fractional entrainment (kg/kg gross liquid flow)
$\widehat{\rho l}$ specific mass of liquid (kg/m^3)
$\widehat{\rho shell}$ specific mass of shell material (kg/m^3)
$\widehat{\rho t}$ specific mass of tray material (kg/m^3)
$\widehat{\rho v}$ specific mass of vapor (kg/m^3)
$\widehat{\sigma}$ surface tension (N/m)

SUBSCRIPTS

sNt set of column trays

AUTHOR CONTRIBUTIONS

Aline R. da Cruz Souza: Conceptualization (supporting); investigation (supporting); methodology (supporting); software (lead); validation (lead); visualization (lead); writing – original draft (equal); writing – review and editing (equal). **Miguel J. Bagajewicz:** Conceptualization (equal); investigation (equal); methodology (equal); supervision (equal); writing – original draft (equal); writing – review and editing (equal). **André Luiz Hemerly Costa:** Conceptualization (equal); investigation (equal); methodology (equal); supervision (equal); writing – original draft (equal); writing – review and editing (equal).

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DATA AVAILABILITY STATEMENT

Data available in article supplementary material.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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