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Nonlinear Model for the Globally Optimal Design of Vertical Vapor Liquid Separation Vessels

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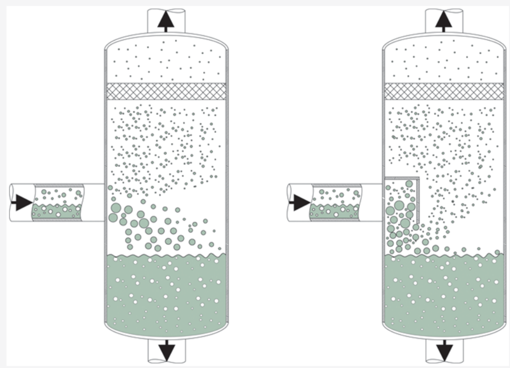
ABSTRACT: Separation vessels are traditionally designed based on rules of thumb that guide the designer to a feasible solution. Despite its widespread use, this approach presents important limitations, which is mostly that there are no concerns about the identification of an optimal solution. Recently, the use of mathematical programming was proposed to solve the design problem of a vertical separation vessel through a mixed-integer linear programming procedure. However, despite the advantages of the mixed-integer linear model, this method has important shortcomings. In this article, we show deficiencies of this linear model and we present a mixed-integer nonlinear model solved using a mixed-integer nonlinear programming procedure. We briefly highlight the importance of using discrete standard values of pipes as well as plates for the design. We also address the use of different recommendations associated to the height of the vessel, thus generating conservative as well as optimistic models and we extend the scope of the design problem to the inclusion of demisters.



■ INTRODUCTION

Vapor−liquid phase separators are used in process plants[1−3] to separate two or more phase streams. For the most part, the critical geometric design variables are the vessel diameter and height or length for vertical and horizontal separators, respectively. The design values for these design variables are found using a series of heuristics procedures/rules/recommendations, such as specified distances around the inlet nozzle as well as liquid residence time to fix the liquid height. Other decisions involve the fluid inlet (nozzle, Schoepentoeter, half-open pipe, etc.), placement of vanes, demisters, vapor outlet nozzles, etc.

The literature about the design of vertical vapor−liquid equilibrium (VLE) separators,[4−6] a heritage from the early years of computerless engineering, still proposes the use of rules of thumb that replace a detailed phenomenological analysis, difficult to make in those early times. For example, there are slenderness ratio limits and/or distances between the inlet nozzle and the top of the vessel or the top of the liquid etc. Other heuristics pertain to design procedures, that is, step by step instructions on how to obtain the values of geometric variables, that is, the basic design. These procedures are usually trial and verification procedures, that is, guesses are made initially and then a verification that the design achieves or exceeds the targeted service performance. This issue was discussed in more detail by Costa and Bagajewicz,[7] where the limitations associated to this traditional approach are outlined.

Aiming at providing more accurate results, computational fluid dynamics (CFD) was also investigated.[8,9] This approach consists of solving an Eulerian−Lagrangian problem (with one phase as a continuous fluid and the other phase as particles) or an Eulerian−Eulerian problem (solving the fluid motion on a specific location in space). Both strategies need a previously proposed vessel design for which they solve the CFD problem. In other words, if one wants an optimal solution, all alternative candidates would have to be explored, which is unpractical, considering the large computing times usually associated to CFD simulations.

In most of the above cases, the heuristics-based and CFD simulation-aided methods are, in essence, a trial-and-verification procedure, that is, the process ends when a suitable design (not necessarily the best possible) is found. It makes sense to think about a "trial-and-improve" procedure, which consists of finding a feasible answer and then improving it until all efforts are exhausted, but that is not recommended in texts.

Breaking the complacency with the widespread trial and verification procedures, Fischer et al.[10] showed that optimal solutions for the vessel design problem based on a mixed-integer linear model (MILM) departed in many cases from the results obtained using heuristics. In this article, the heuristics procedure to design vertical separation vessels were reviewed

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and a MILM was proposed and solved using a mixed-integer linear programming (MILP) procedure or simple enumeration.

Usually, a critical size of the droplets above which they will not be carried by the vapor is used as basis for the design. It is therefore important to be able to determine the settling velocity for the given operating conditions more accurately. The typical approach used by Fischer et al.,[10] which follows some of the practices in the literature,[4,6,11] uses a single constant ($\hat{K}_v$) to simplify the balance of buoyancy, gravitational, and drag forces over droplets. This assumption allows a simpler mathematical problem, but it leads to important accuracy limitations.

Therefore, we present a nonlinear formulation of the vessel design problem that presents a more accurate representation of the system behavior, where the drag coefficient depends on the Reynolds number. We also explore the influence of the critical droplet diameter, the effect of adding a demister, and the liquid residence time. Finally, we propose optimistic and pessimistic nonlinear models for any practitioner that may wonder about the validity of certain assumptions.

Our article is organized as follows: We first present a summary of the phase separator design equations and then we compare solutions of the nonlinear model proposed with heuristics solutions and those obtained using previous linear models. We omit discussing several practical considerations, such as heat losses, inlet devices, entrainment efficiency, aspects that we have left for future work.

■ DESIGN EQUATIONS AND HEURISTICS

The design variables of a vertical separator are: diameter, height, type of top and bottom headers, and wall thickness (Figure 1). The vessel can be constructed using standard pipes

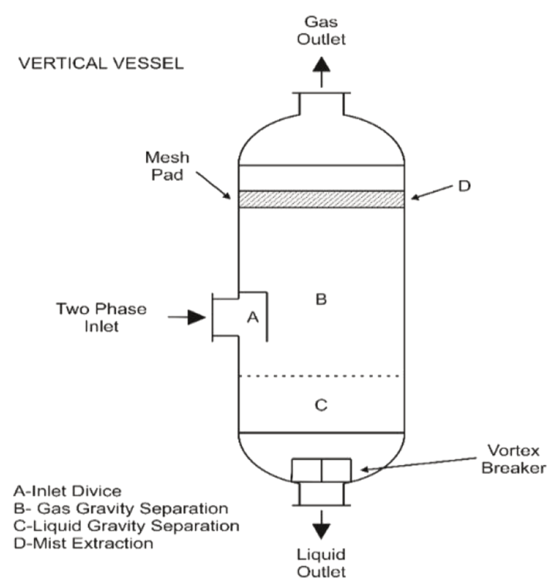

Figure 1. Vertical phase separator.

or, for large diameters, rolled and welded plates as well as ellipsoidal or hemispherical top and bottom. The thickness is always subject to pressure constraints. Other additional design decision variables are: mist extractor/eliminator or demister, vortex breaker for the liquid outlet, and inlet and outlet deflection devices, where the work of Wood[12] proposed interesting thoughts.

The literature present heuristic procedures to obtain the major design variables,[4−6] without any explicit concern about attaining an optimal solution.

We now discuss the differences among the mentioned heuristics, the linear model and the appropriate modeling (model parameters are represented with a "^" on the top) in relation to:

Minimum Vessel Diameter.

$$D_{\text{vessel}} = \left(\frac{4\hat{Q}_v}{\pi v_v}\right)^{1/2} \tag{1}$$

where $\hat{Q}_v$ is the operating volumetric flow rate of the vapor, D_{vessel} is the vessel diameter, and v_v is the terminal velocity. For smaller diameters, such that regular scheduled pipes can be used, authors suggest rounding off the diameter to the next available commercial diameter.

Terminal Velocity. The terminal velocity (or settling velocity) (v_v) of a droplet of a certain size ($\hat{d}_{\text{d, crit}}$) is used in eq 1. Thus,

$$v_v = \left(\frac{4\,\hat{d}_{\text{d,crit}}\hat{g}}{3\,C_D}\right)^{1/2}\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)^{1/2} \tag{2}$$

where C_D is the drag coefficient.[4,13,14] Typically, the above formula is rewritten introducing the coefficient K_v:

$$v_v = K_v\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)^{1/2} \tag{3}$$

The physical behavior of the drag force between the droplet and the surrounding vapor phase implies that the C_D also depends on the Reynolds number $\left(R_e = \frac{\hat{\rho}_v\,\hat{d}_{\text{d,crit}}\,v_v}{\hat{\mu}_v}\right)$. For example, Stewart and Arnold[13] proposed:

$$C_D = \frac{24}{R_e} + \frac{3}{R_e^{0.5}} + 0.34 \tag{4}$$

There are Other Formulas. The GPSA Engineering Databook,[15] for example, uses a simpler formula $C_D = 1.31\ 10^7 \hat{\rho}_v \hat{d}_{\text{d,crit}}^{\ 3}(\hat{\rho}_l - \hat{\rho}_v)/\hat{\mu}^2$, where $\hat{\mu}$ in cp; $\hat{\rho}$ in lb./ft,^{3} and $\hat{d}_{\text{d, crit}}$ in ft.

Despite the dependence between C_D and the Reynolds number, some authors adopted a fixed value for the coefficient K_v.[4,6,11] This representation was also used by Fischer et al.[10] in their linear model. Watkins[16] and Blackwell[17] also ignored the dependence with the Reynolds number but proposed models for evaluation of $\hat{K}_v$ as a function of $\hat{F}_{lv} = (\hat{W}_l/\hat{W}_v)\sqrt{\hat{\rho}_v/\hat{\rho}_l}$ ($\hat{W}_v$ and $\hat{W}_l$ are the vapor and liquid mass flowrates, respectively). Aiming to provide a solution with higher accuracy, we use in this article the rigorous determination of C_D in relation to the Reynolds number.

Demister. When a demister is used, the calculation of the vapor velocity does not depend on the original size of the droplets; it depends on the effectiveness of the demister in the coalescence of the droplets and therefore small velocities that lead to higher diameters are no longer needed. Indeed, demisters coalesce the small droplets into larger droplets, which have higher settling velocity. The mechanism involves the droplet collision and adherence to a target, coalescence into larger droplets, and drainage down. Demisters of the

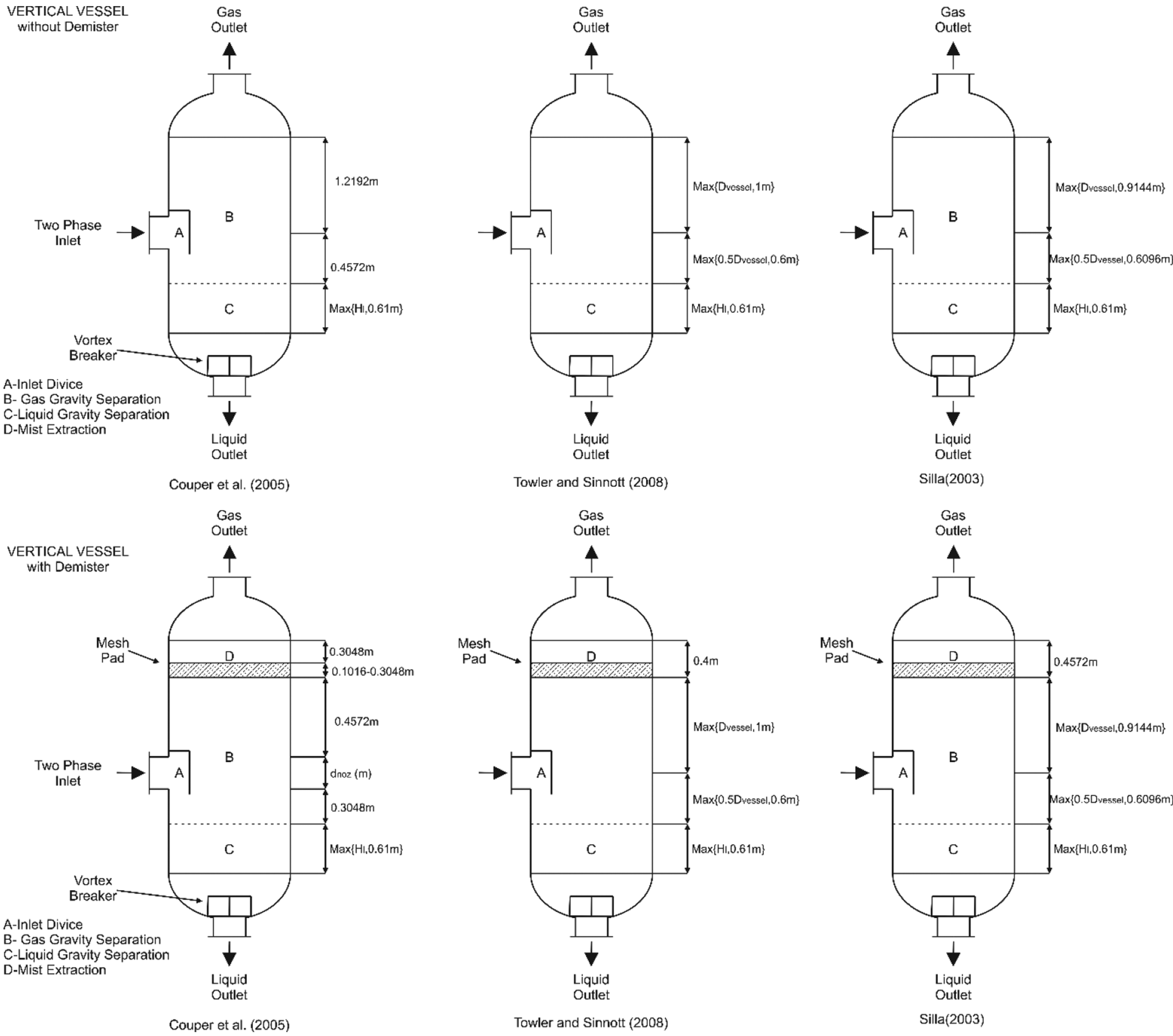

Figure 2. H_v values selected for the different heuristics.

impingement type are the most common in industry. The impingement types are divided in baffles (vanes or plates) or wire mesh types devices. The wire mesh types are also divided in woven or knitted types. There are other types such as microfiber, centrifugal, coalescing pack. However, the knitted types are the standard in the industry. Thus, when there is a demister, ad-hoc values for $\hat{K}_v$ are used: Datta[14] lists different values for different commercial demisters, from 0.107 to 0.198, not related to $\hat{F}_{lv}$.

Vapor Height. In this article we use the expressions developed by three references, that is:

$$H_v = 1.6764 \quad \text{Couper et al.}^{5} \tag{5}$$

$$H_v = \text{Max}\{0.5\, D_{vessel},\, 0.6\text{ m}\} + \text{Max}\{D_{vessel},\, 1\text{ m}\} \quad \text{Towler and Sinnott}^{6} \tag{6}$$

$$H_v = \text{Max}\{0.5\, D_{vessel},\, 0.6096\text{ m}\} + \text{Max}\{D_{vessel},\, 0.9144\text{ m}\} \quad \text{Silla}^{4} \tag{7}$$

where the first term in eqs 6 and 7 is the distance between the liquid surface and the center of the inlet nozzle ($H_{inlet-liq}$) and the second term is the height between the center of the inlet nozzle and the upper tangent line, called disengagement height ($H_{disengage}$). We summarize the different choices in Figure 2 and generalize these expressions later for the presence of a demister.

Liquid Level. It is obtained using a given residence time, $\hat{t}_s$, subject to a lower limit.

$$H_l = \text{Max}\left\{\frac{4\hat{Q}_l\hat{t}_s}{\pi D_{vessel}^2},\, \hat{H}_{l,min}\right\} \tag{8}$$

Total Height of the Vessel. It is obtained by adding the vapor and liquid heights, that is:

$$H_{vessel} \geq H_l + H_v \tag{9}$$

Slenderness. The H_{vessel}/D_{vessel} bounds (between 3 and 5) can have a significant impact on the design (this discussion can be traced back to Watkins[16]). In turn, ASME[18] does not

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mention a restriction on H_{vessel}/D_{vessel}, but it discusses buckling of circular sections recommending a minimum thickness to diameter ratio. Our formulas are good for $t/D < 0.25$ (ASME[18]) and our data always comply. Therefore, according to the heuristics, the designer must apply the guideline: if $H_{vessel}/D_{vessel} > 5$, then the diameter is increased a certain percentage until it complies and the height adjusted again. In turn, if $H_{vessel}/D_{vessel} < 3$, then the height is increased keeping the diameter constant.

Wall Thickness of Shell and Heads. The choices are hemispherical or ellipsoidal heads. The thickness is given by:

$$t_{shell} = \text{Max}\left\{\frac{\hat{P}\frac{D_{vessel}}{2}}{\hat{S}\hat{E} - 0.6\hat{P}}, \hat{t}_{min}\right\} \quad (10)$$

$$t_{h-ellipsoidal} = \text{Max}\left\{\frac{\hat{P}D_{vessel}}{2\hat{S}\hat{E} - 0.2\hat{P}}, \hat{t}_{min}\right\} \quad (11)$$

$$t_{h-hemispherical} = \text{Max}\left\{\frac{\hat{P}.\frac{D_{vessel}}{2}}{2\hat{S}\hat{E} - 0.2\hat{P}}, \hat{t}_{min}\right\} \quad (12)$$

where $\hat{P}$ is the maximum vessel pressure difference, $\hat{S}$ is the allowable tensile strength, and $\hat{E}$ the joint efficiency.

Vessel Material Volume. The volume of the shell material and the volume of the head material are obtained by volume difference as follows:

$$V_{shell} = \frac{\pi}{4}\{(D_{vessel} + 2t_{shell})^2 - D_{vessel}^2\}H_{vessel} = \pi(D_{vessel}t_{shell} + t_{shell}^2)H_{vessel} \quad (13)$$

$$V_{head} = \frac{\pi}{12}(6D_{vessel}^2 t_h + 12D_{vessel}t_h^2 + 8t_h^3) \quad \text{(for ellipsoidal head)} \quad (14)$$

$$V_{head} = \frac{\pi}{6}(6D_{vessel}^2 t_h + 12D_{vessel}t_h^2 + 8t_h^3) \quad \text{(for hemispherical head)} \quad (15)$$

Separation vessels can be constructed using standardized pipes or plates with standard thickness. If plates are used, there are recommendations to round up to the next standard diameter value.[4,5] Therefore, the diameter used for plates is also discrete.

Cost. We use the cost of the metal plus the cost of the demister. The cost of the metal is straightforward. In turn, demister suppliers sell them using mass ($\hat{C}_{dem,\,kg}$ (US\$/kg)) or the transversal area of the demister ($\hat{C}_{dem,\,m^2}$ (US\$/m^2)). In this article, we do not add other costs, like labor, logistics, manufacturing overheads. The assumption made in this article is that the cost of labor and logistic is the same irrespective of the vessel size.

Finally, we offer the following additional thoughts:

- We do not consider in the modeling the presence of bubbles in the liquid and the corresponding vapor entrainment in the outgoing liquid, a condition that is seldom discussed, if at all.
- The impact of the diameter on liquid and vapor entrainment and the use of a demister needs to be revisited focusing on a relationship of drop size distribution with entrainment, these discussions are left for future work.

OPTIMIZATION MODEL

We now present a mixed-integer nonlinear model (MINLM) that we propose solving using mathematical programming. We introduce a binary variable (z_{dem}) to indicate the presence of a demister that was not considered by Fischer et al.[10] and can bring important cost reductions in certain situations. There are also binary variables (z_{he} and z_{hh}) used for the choice between ellipsoidal and hemispherical heads. We also introduce the variable $v_{v,C}$ for the terminal velocity without demister. The resulting model is:

$$\text{Min Cost} = (V_{shell} + 2\,V_{head})\hat{\rho}_{steel}\hat{C}_{steel} + z_{dem}V_{dem}\hat{\rho}_{dem}\hat{C}_{dem} \quad (16)$$

s.t.

$$v_v = (1 - z_{dem})v_{v,C} + \hat{K}_{v,dem}\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)^{1/2} z_{dem} \quad (17)$$

$$\left[\frac{24\hat{\mu}v_{v,C}}{\hat{\rho}_v\hat{d}_{d,crit}} + \left(\frac{\hat{\mu}}{\hat{\rho}_v\hat{d}_{d,crit}}\right)^{0.5} 3v_{v,C}^{\ 1.5} + 0.34\,v_{v,C}^{\ 2} - \left(\frac{4\hat{d}_{d,crit}\hat{g}}{3}\right)\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)\right] = 0 \quad (18)$$

$$D_{vessel} \geq \left(\frac{4\hat{Q}_v}{\pi v_v}\right)^{1/2} \quad (19)$$

$$D_{vessel} \geq \hat{d}_{min} \quad (20)$$

$$H_l \geq \frac{4\hat{Q}_l\hat{t}_s}{\pi D_{vessel}^2} \quad (21)$$

$$H_l \geq \hat{H}_{l\_min} \quad (22)$$

$$H_{vessel} \geq H_l + H_v \quad (23)$$

$$H_v = \begin{cases} 1.6764\,(1 - z_{dem}) + (1.0668 + \hat{d}_{noz} + \hat{H}_{dem})z_{dem} \quad \text{(Couper et al.}^{5}\text{)} \\ (H_{inlet-liq} + H_{disengage} + 0.4\,\hat{z}z_{dem}) \quad \text{(Towler and Sinnott}^{6}\text{)} \\ (H_{inlet-liq} + H_{disengage} + 0.4572z_{dem}) \quad \text{(Silla}^{4}\text{)} \end{cases} \quad (24)$$

$$H_{inlet-liq} \geq \begin{cases} \text{Max}\{0.5D_{vessel}, 0.6\text{ m}\} \quad \text{(Towler and Sinnott}^{6}\text{)} \\ \text{Max}\{0.5D_{vessel}, 0.6096\text{ m}\} \quad \text{(Silla}^{4}\text{)} \end{cases} \quad (25)$$

$$H_{disengage} \geq \begin{cases} \text{Max}\{D_{vessel}, 1\text{ m}\} \quad \text{(Towler and Sinnott}^{6}\text{)} \\ \text{Max}\{D_{vessel}, 0.9144\text{ m}\} \quad \text{(Silla}^{4}\text{)} \end{cases} \quad (26)$$

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$$3 \le H_{\text{vessel}}/D_{\text{vessel}} \le 5 \quad (27)$$

$$t_{\text{shell}} \ge \frac{\hat{P}\frac{D_{\text{vessel}}}{2}}{\hat{S}\hat{E} - 0.6\hat{P}} \quad (28)$$

$$t_{\text{shell}} \ge \hat{t}_{\min} \quad (29)$$

$$t_{\text{h}} \ge \frac{\hat{P}\, D_{\text{vessel}}}{2\hat{S}\hat{E} - 0.2\hat{P}} z_{\text{he}} + \frac{\hat{P}\frac{D_{\text{vessel}}}{2}}{2\hat{S}\hat{E} - 0.2\hat{P}} z_{\text{hh}} \quad (30)$$

$$t_{\text{h}} \ge \hat{t}_{\min} \quad (31)$$

$$V_{\text{shell}} = \pi(D_{\text{vessel}}t_{\text{shell}} + t_{\text{shell}}^2)H_{\text{vessel}} \quad (32)$$

$$V_{\text{head}} = \frac{\pi}{12}(6D_{\text{vessel}}^2 t_{\text{h}} + 12D_{\text{vessel}}t_{\text{h}}^2 + 8t_{\text{h}}^3)z_{\text{he}} + \frac{\pi}{6}(6D_{\text{vessel}}^2 t_{\text{h}} + 12\, D_{\text{vessel}}t_{\text{h}}^2 + 8t_{\text{h}}^3)z_{\text{hh}} \quad (33)$$

$$z_{\text{he}} + z_{\text{hh}} = 1 \quad (34)$$

$$V_{\text{dem}} = \hat{h}_{\text{dem}}\frac{\pi}{4}D_{\text{vessel}}^2 \quad (35)$$

In this model, $\hat{d}_{\text{noz}}$ is the diameter of the inlet nozzle, in turn obtained using a velocity $\hat{u}_{\text{n}}$ (inlet nozzle velocity) within specified limits, that is, $60\sqrt{\hat{\rho}_{\text{mix}}} \le \hat{u}_{\text{n}}(\text{ft/s}) \le 100\sqrt{\hat{\rho}_{\text{mix}}}$, as proposed by Couper et al.[5] In our models, we chose the conservative value of $90\sqrt{\hat{\rho}_{\text{mix}}}$.

■ MODEL REFORMULATION

The reformulation explores the discrete nature of some design variables to eliminate nonlinearities and was also explored before successfully for different thermal equipment.[7]

Several variables that are discrete in nature are represented formally as follows:

$$D_{\text{vessel}} = \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \quad (36)$$

$$t_{\text{shell}} = \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std},t_{\text{shell}}}\, y\text{vessel}_{\text{std}} \quad (37)$$

$$t_{\text{h}} = \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}}\, y\text{vessel}_{\text{std}} \quad (38)$$

$$\sum_{\text{std}=1}^{\text{stdmax}} y\text{vessel}_{\text{std}} = 1 \quad (39)$$

where $\widehat{\text{Vessel}}_{\text{std, intd}}$, $\widehat{\text{Vessel}}_{\text{std}, t_{\text{shell}}}$, and $\widehat{\text{Vessel}}_{\text{std, th}}$ are parameters which represent the commercial alternatives of inner diameter, shell thickness, and head thickness, respectively. The resulting MINLM model is:

$$\text{Min Cost} = \text{Mass}\sum_{\text{std}}^{\text{stdmax}} \hat{C}_{\text{steel,std}}\, y\text{vessel}_{\text{std}} + z_{\text{dem}}V_{\text{dem}}\hat{\rho}_{\text{dem}}\hat{C}_{\text{dem}} \quad (40)$$

s.t.

$$\text{Mass} = (V_{\text{shell}} + 2\, V_{\text{head}})\hat{\rho}_{\text{steel}} \quad (41)$$

$$v_{\text{v}} = (1 - z_{\text{dem}})v_{\text{v,C}} + \hat{K}_{\text{v,dem}}\left(\frac{\hat{\rho}_{\text{l}} - \hat{\rho}_{\text{v}}}{\hat{\rho}_{\text{v}}}\right)^{1/2} z_{\text{dem}} \quad (42)$$

$$\left[\frac{24\hat{\mu}v_{\text{v,C}}}{\hat{\rho}_{\text{v}}\hat{d}_{\text{d,crit}}} + \left(\frac{\hat{\mu}}{\hat{\rho}_{\text{v}}\hat{d}_{\text{d,crit}}}\right)^{0.5} 3v_{\text{v,C}}^{1.5} + 0.34\, v_{\text{v,C}}^{2} - \left(\frac{4\hat{d}_{\text{d,crit}}\hat{g}}{3}\right)\left(\frac{\hat{\rho}_{\text{l}} - \hat{\rho}_{\text{v}}}{\hat{\rho}_{\text{v}}}\right)\right] = 0 \quad (43)$$

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \ge \left(\frac{4\hat{Q}_{\text{v}}}{\pi v_{\text{v}}}\right)^{1/2} \quad (44)$$

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \ge \hat{d}_{\min} \quad (45)$$

$$H_{\text{l}} \ge \frac{4\hat{Q}_{\text{l}}\hat{t}_{\text{s}}}{\pi}\sum_{\text{std}=1}^{\text{stdmax}} \frac{y\text{vessel}_{\text{std}}}{\widehat{\text{Vessel}}_{\text{std,intd}}^2} \quad (46)$$

$$H_{\text{l}} \ge \hat{H}_{\text{l\_min}} \quad (47)$$

$$H_{\text{vessel}} \ge H_{\text{l}} + H_{\text{v}} \quad (48)$$

$$H_{\text{v}} = \begin{cases} 1.6764\,(1 - z_{\text{dem}}) + (1.0668 + \hat{d}_{\text{noz}} + \hat{h}_{\text{dem}})z_{\text{dem}} \\ \quad \text{(Couper et al.[5])} \\ (H_{\text{inlet-liq}} + H_{\text{disengage}} + 0.4\, z_{\text{dem}}) \\ \quad \text{(Towler and Sinnott[6])} \\ (H_{\text{inlet-liq}} + H_{\text{disengage}} + 0.4572\, z_{\text{dem}}) \quad \text{(Silla[4])} \end{cases} \quad (49)$$

$$H_{\text{inlet-liq}} \ge 0.5\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \quad \text{(Towler and Sinnot[6] and Silla[4])} \quad (50)$$

$$H_{\text{inlet-liq}} \ge 0.6\text{ m} \quad \text{(Towler and Sinnot[6])} \quad (51)$$

$$H_{\text{inlet-liq}} \ge 0.6096\text{ m (Silla[4])} \quad (52)$$

$$H_{\text{disengage}} \ge \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \quad \text{(Towler and Sinnot[6] and Silla[4])} \quad (53)$$

$$H_{\text{disengage}} \ge 1\text{ m (Towler and Sinnot[6])} \quad (54)$$

$$H_{\text{disengage}} \ge 0.9144\text{ m (Silla[4])} \quad (55)$$

$$\sum_{\text{stdmax}}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \ge \hat{d}_{\min} \quad (56)$$

$$H_{\text{vessel}} \ge 3\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}\, y\text{vessel}_{\text{std}} \quad (57)$$

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$$H_{\text{vessel}} \leq 5 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} y\text{vessel}_{\text{std}} \tag{58}$$

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std},t_{\text{shell}}} y\text{vessel}_{\text{std}} \geq \frac{\hat{P} \cdot \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \cdot y\text{vessel}_{\text{std}}}{2(\hat{S}\hat{E} - 0.6\hat{P})} \tag{59}$$

$$\sum_{\text{std}}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std},t_{\text{shell}}} y\text{vessel}_{\text{std}} \geq \hat{t}_{\min} \tag{60}$$

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} y\text{vessel}_{\text{std}} \geq \frac{\hat{P} \sum_{\text{std}}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \cdot y\text{vessel}_{\text{std}}}{2\hat{S}\hat{E} - 0.2\hat{P}} z_{\text{he}} + \frac{\hat{P} \sum_{\text{std}=1}^{\text{stdmax}} \frac{\widehat{\text{Vessel}}_{\text{std,intd}}}{2} \cdot y\text{vessel}_{\text{std}}}{2\hat{S}\hat{E} - 0.2\hat{P}} z_{\text{hh}} \tag{61}$$

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} y\text{vessel}_{\text{std}} \geq \hat{t}_{\min} \tag{62}$$

$$z_{\text{he}} + z_{\text{hh}} = 1 \tag{63}$$

$$V_{\text{shell}} = \pi \left(\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \widehat{\text{Vessel}}_{\text{std},t_{\text{shell}}} y\text{vessel}_{\text{std}} + \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^2_{\text{std},t_{\text{shell}}} y\text{vessel}_{\text{std}} \right) H_{\text{vessel}} \tag{64}$$

$$\begin{aligned} V_{\text{head}} = \frac{\pi}{12} \Bigg\{ & 6 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} \widehat{\text{Vessel}}^2_{\text{std,intd}} y\text{vessel}_{\text{std}} + 12 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \widehat{\text{Vessel}}^2_{\text{std,th}} y\text{vessel}_{\text{std}} + 8 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^3_{\text{std,th}} y\text{vessel}_{\text{std}} \Bigg\} z_{\text{he}} \\ + \frac{\pi}{6} \Bigg\{ & 6 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} \widehat{\text{Vessel}}^2_{\text{std,intd}} y\text{vessel}_{\text{std}} + 12 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \widehat{\text{Vessel}}^2_{\text{std,th}} \, y\text{vessel}_{\text{std}} + 8 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^3_{\text{std,th}} y\text{vessel}_{\text{std}} \Bigg\} z_{\text{hh}} \end{aligned} \tag{65}$$

$$V_{\text{dem}} = \hat{h}_{\text{dem}} \frac{\pi}{4} \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^2_{\text{std,intd}} y\text{vessel}_{\text{std}} \tag{66}$$

We recognize that pipes and rolled plates have different costs, hence the cost is indexed with std. The above model is nonlinear and it also contains products of binary variables and products of binary variables and continuous variables, as well as truly nonlinear equations. Thus, we reformulate these equations. Equation 61 is replaced by:

$$\sum_{\text{stdmax}}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} y\text{vessel}_{\text{std}} \geq \frac{\hat{P} \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}}{2 \cdot \hat{S}\hat{E} - 0.2\hat{P}} \text{wvesszhe}_{\text{std,he}} + \frac{\hat{P} \cdot \sum_{\text{std}=1}^{\text{stdmax}} \frac{\widehat{\text{Vessel}}_{\text{std,intd}}}{2}}{2\hat{S}\hat{E} - 0.6\hat{P}} \text{wvesszhh}_{\text{std,hh}} \tag{67}$$

$$\text{wvesszhe}_{\text{std,he}} \leq y\text{vessel}_{\text{std}} \tag{68}$$

$$\text{wvesszhe}_{\text{std,he}} \leq z_{\text{he}} \tag{69}$$

$$\text{wvesszhe}_{\text{std,he}} \geq y\text{vessel}_{\text{std}} + z_{\text{he}} - 1 \tag{70}$$

$$\text{wvesszhh}_{\text{std,hh}} \leq y\text{vessel}_{\text{std}} \tag{71}$$

$$\text{wvesszhh}_{\text{std,hh}} \leq z_{\text{hh}} \tag{72}$$

$$\text{wvesszhh}_{\text{std,hh}} \geq y\text{vessel}_{\text{std}} + z_{\text{hh}} - 1 \tag{73}$$

Equation 64 is replaced by:

$$V_{\text{shell}} = \pi \left(\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \widehat{\text{Vessel}}_{\text{std},t_{\text{shell}}} + \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^2_{\text{std},t_{\text{shell}}} \right) \text{whvessel}_{\text{std}} \tag{74}$$

$$\text{whvessel}_{\text{std}} - \widehat{\Gamma}_{\text{h}} y\text{vessel}_{\text{std}} \leq 0 \tag{75}$$

$$\text{whvessel}_{\text{std}} \geq 0 \tag{76}$$

$$(H_{\text{vessel}} - \text{whvessel}_{\text{std}}) - \widehat{\Gamma}_{\text{h}}(1 - y\text{vessel}_{\text{std}}) \leq 0 \tag{77}$$

$$(H_{\text{vessel}} - \text{whvessel}_{\text{std}}) \geq 0 \tag{78}$$

In turn, eq 65 is reformulated as follows:

$$\begin{aligned} V_{\text{head}} = \frac{\pi}{12} \Bigg(& 6 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} \widehat{\text{Vessel}}^2_{\text{std,intd}} + 12 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \widehat{\text{Vessel}}^2_{\text{std,th}} + 8 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^3_{\text{std,th}} \Bigg) \text{wvesszhe}_{\text{std,he}} \\ + \frac{\pi}{6} \Bigg(& \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,th}} \widehat{\text{Vessel}}^2_{\text{std,intd}} + 12 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}} \widehat{\text{Vessel}}^2_{\text{std,th}} + 8 \sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}^3_{\text{std,th}} \Bigg) \text{wvesszhh}_{\text{std,hh}} \end{aligned} \tag{79}$$

Finally, the objective function (40) is reformulated as follows:

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$$\text{Min Cost} = \sum_{\text{std}=1}^{\text{stdmax}} w\text{mass}_{\text{std}}\hat{C}_{\text{steel,std}} + z_{\text{dem}}V_{\text{dem}}\hat{\rho}_{\text{dem}}\hat{C}_{\text{dem}} \tag{80}$$

$$w\text{mass}_{\text{std}} - \widehat{\Gamma_w} y\text{vessel}_{\text{std}} \leq 0 \tag{81}$$

$$w\text{mass}_{\text{std}} \geq 0 \tag{82}$$

$$(\text{Mass} - w\text{mass}_{\text{std}}) - \widehat{\Gamma_w}(1 - y\text{vessel}_{\text{std}}) \leq 0 \tag{83}$$

$$(\text{Mass} - w\text{mass}_{\text{std}}) \geq 0 \tag{84}$$

The linearization of products of z_{dem} and V_{dem} is standard. Equation 42 is replaced by:

$$v_v = (v_{v,C} - wvz_{v,C,\text{dem}}) + \hat{K}_{v,\text{dem}}\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)^{1/2} z_{\text{dem}} \tag{85}$$

$$wvz_{v,C,\text{dem}} - \widehat{\Gamma_w}\, z_{\text{dem}} \leq 0 \tag{86}$$

$$wvz_{v,C,\text{dem}} \geq 0 \tag{87}$$

$$(v_{v,C} - wvz_{v,C,\text{dem}}) - \widehat{\Gamma_w}(1 - y\text{vessel}_{\text{std}}) \leq 0 \tag{88}$$

$$(v_{v,C} - wvz_{v,C,\text{dem}}) \geq 0 \tag{89}$$

This full mixed-integer nonlinear programming (MINLP) model, with only a few nonlinear equations, can be solved using local solvers (e.g., SBB and DICOPT); we also run it using BARON, ANTIGONE, and RYSIA (bound contraction; Faria and Bagajewicz[19]). Because RYSIA is not commercial, we add details of the relaxed model used to build its lower bound. An aspect that must be noted in the model above is if we assume a constant value of K_v, then the model becomes a linear one, i.e., an MILP problem.[19]

The relaxed model that RYSIA requires partitioning of $v_{v,C}$ and the reformulation of the equations where it participates. We show the equations for the partitioning first.

$$\widehat{vs}_s = vs^L + (\text{ord}(s) - 1)\frac{vs^U - vs^L}{\text{card}(S) - 1} + \tag{90}$$

$$\sum_{s\in S} yvs_s\widehat{vs}_s \leq v_{v,C} \leq \sum_{s\in S} yvs_s\widehat{vs}_{s+1} \tag{91}$$

$$\sum_{s\in S} yvs_s = 1 \tag{92}$$

where yvs_s is a binary variable. Equation 90 defines a parameter, and eqs 91 and 92 require that $v_{v,C}$ is confined to one and only one partition.

The following equations are the relaxation of eq 43:

$$\frac{24\hat{\mu}}{\hat{\rho}_v\hat{d}_{d,\text{crit}}}v_{v,C} + \sum_{s\ni S}\left[3\left(\frac{\hat{\mu}}{\hat{\rho}_v\hat{d}_{d,\text{crit}}}\right)^{0.5}\widehat{vs}_s^{1.5} + 0.34\,\widehat{vs}_s^{2}\right]yvs_s - \left(\frac{4\hat{d}_{d,\text{crit}}\hat{g}}{3}\right)\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right) \leq 0 \tag{93}$$

$$\frac{24\hat{\mu}}{\hat{\rho}_v\hat{d}_{d,\text{crit}}}v_{v,C} + \sum_{s\ni S}\left[3\left(\frac{\hat{\mu}}{\hat{\rho}_v\hat{d}_{d,\text{crit}}}\right)^{0.5}\widehat{vs}_{s+1}^{1.5} + 0.34\,\widehat{vs}_{s+1}^{2}\right]yvs_s - \left(\frac{4\hat{d}_{d,\text{crit}}\hat{g}}{3}\right)\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right) \geq 0 \tag{94}$$

We now rewrite eq 44 replacing v_v by its expression given by eq 42:

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}y\text{vessel}_{\text{std}} \geq \left(\frac{4\hat{Q}_v}{\pi}\right)^{1/2}\left[\frac{(1 - z_{\text{dem}})}{v_{v,C}^{0..5}} + \frac{z_{\text{dem}}}{\left[\hat{K}_{v,\text{dem}}\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)^{1/2}\right]^{1/2}}\right] \tag{95}$$

In turn, we relax the equation as follows:

$$\sum_{\text{std}=1}^{\text{stdmax}} \widehat{\text{Vessel}}_{\text{std,intd}}y\text{vessel}_{\text{std}} \geq \left(\frac{4\cdot\hat{Q}_v}{\pi}\right)^{1/2}\left[\sum_{s\ni S}\frac{(yvs_s - wyvsz_{s,\text{dem}})}{\widehat{vs}_{s+1}^{0.5}} + \frac{z_{\text{dem}}}{\left[\hat{K}_{v,\text{dem}}\left(\frac{\hat{\rho}_l - \hat{\rho}_v}{\hat{\rho}_v}\right)^{1/2}\right]^{1/2}}\right] \tag{96}$$

$$wyvsz_{s,\text{dem}} \leq yvs_s \tag{97}$$

$$wyvsz_{s,\text{dem}} \leq z_{\text{dem}} \tag{98}$$

$$wyvsz_{s,\text{dem}} \geq yvs_s + z_{\text{dem}} - 1 \tag{99}$$

The resulting relaxed model is linear and is a lower bound of the problem. RYSIA uses this model to obtain a global optimum.

■ RESULTS

Aside from showing results for our example and highlight the differences with results from an MILP model, we explore different aspects of the problem: the effect of the critical droplet size, the liquid residence time, the utilization of demisters, and a discussion related to conservative and optimistic models.

The discrete values of the diameter and thickness for pipes used in our examples are given in Table 1. Without loss of generality, we only use STD, XS, and XXS and we do not include schedules 10, 40, and 60. For diameters higher than 60 inches, we used rolled steel plates discretizing the external diameter using 2 inches steps, and thickness as shown in Table 2. We use $\hat{\rho}_{\text{steel}}$ = 7900 kg/m^3 for ASTM SA516 G70 (we dismiss the difference between the density of carbon and stainless steels), $\hat{C}_{\text{steel}}$ = 0.65 US$/kg for raw steel, $\hat{C}_{\text{stainless - steel}}$ = 2.85US$/kg for stainless steel. For plates, we add 10% to the cost, to consider rolling and welding. We use RYSIA in a simplified form as the global solver. Indeed, we use sufficient intervals for partitioning so that the first lower bound solution and the upper bound calculated using its results exhibit a very small gap.

The example investigated was taken from Towler and Sinnott.[6] It consists of water and steam in equilibrium at 4 bar, according to the description shown in Table 3. The design

Table 1. Pipe Data

nominal diameter (in)	inner diameter (m)	thickness (m)	nominal diameter (in)	inner diameter (m)	thickness (m)
6-XXS	0.1244	0.02195	22-STD	0.5399	0.00953
6-XS	0.1464	0.01097	24-XS	0.5846	0.0127
6-STD	0.1541	0.00711	24-STD	0.5909	0.00953
8-XXS	0.1746	0.02223	26-XS	0.6346	0.0127
8-XS	0.1937	0.0127	26-STD	0.6409	0.00953
8-STD	0.2027	0.00818	28-XS	0.6856	0.0127
10-XXS	0.2222	0.0254	28-STD	0.6919	0.00953
10-XS	0.2476	0.0127	30-XS	0.7366	0.0127
10-STD	0.2545	0.00927	30-STD	0.7429	0.00953
12-XXS	0.2730	0.0254	32-XS	0.7876	0.0127
12-XS	0.2984	0.0127	32-STD	0.7939	0.00953
12-STD	0.3048	0.00952	34-XS	0.8386	0.0127
14-XS	0.3302	0.0127	34-STD	0.8448	0.00953
14-STD	0.3365	0.00953	36-XS	0.8886	0.0127
16-XS	0.3810	0.0127	36-STD	0.8949	0.00953
16-STD	0.3873	0.00953	42-XS	1.0416	0.0127
18-XS	0.4316	0.0127	42-STD	1.0479	0.00953
18-STD	0.4379	0.00953	48-XS	1.1936	0.0127
20-XS	0.4826	0.0127	48-STD	1.1999	0.00953
20-STD	0.4889	0.00953	60-XS	1.4986	0.0127
22-XS	0.5336	0.0127	60-STD	1.5049	0.00953

Table 2. Standard Plate Thickness

(inch)	(mm)	(inch)	(mm)
1/8	3.18	1 3/8	34.93
5/32	3.97	1 1/2	38.10
3/16	4.76	1 3/4	44.45
1/4	6.35	2	50.80
5/16	7.94	2 1/4	57.15
3/8	9.53	2 1/2	63.50
7/16	11.11	2 3/4	69.85
1/2	12.70	3	76.20
9/16	14.29	3 1/2	88.90
5/8	15.88	4	101.60
3/4	19.05	4 1/2	114.30
7/8	22.23	5	127.00
1	25.40	6	152.40
1 1/8	28.58		
1 1/4	31.75		

pressure is 1.10 times the expected operating pressure or the expected operating pressure (43.32 psig) plus 25 psi, whichever is greater.

For a given separation task, we compare the results obtained using the proposed approach with previous results from the literature, encompassing heuristics[6] and optimization using linear models.[10] Both approaches from the literature are based on the use of a fixed $\hat{K}_v$.

Table 3. Data for Example

parameter	value	parameter	value
$\hat{Q}_v$(m^3/s)	0.257	$\hat{\mu}_v$(Pa s)	$1.45207 \cdot 10^{-5}$
$\hat{Q}_l$(m^3/s)	0.0003	$\hat{t}_s$(s)	750
$\hat{\rho}_l$(kg/m^3)	926.4	$\hat{P}$(psig)	68.32
$\hat{\rho}_v$(kg/m^3)	2.16	$\hat{S}$(psi)	17500
$\hat{d}_{d,\ crit}$(μm)	200	$\hat{E}$	1

The results obtained using the proposed approach are shown in Table 4, considering different models. In Table 5,

Table 4. MINLM Results Considering Different Models

model/variables	Couper et al.[5]	Towler and Sinnott[6]	Silla[4]
D_{vessel} (m)	0.6919	0.6919	0.6919
H_{vessel} (m)	2.2864	2.2100	2.1340
$\hat{K}_v$ (m/s)	0.0354	0.0354	0.0354
head type	ellipsoidal	ellipsoidal	ellipsoidal
mass (kg)	495.70	483.02	470.41

Table 5. Results for Towler and Sinnott[6] for Heuristics and the MILM for Different Values of K_v

MODEL/ variables	Towler and Sinnott[6] results	heuristic $\hat{K}_v$ by Blackwell[17]	MILP $\hat{K}_v$ by Blackwell[17]	MILP $\hat{K}_v$ = 0.0105 (same as Towler and Sinnot[6])
D_{vessel} (m)	1.25	0.5399	0.3873	1.5049
H_{vessel}(m)	3.75	2.3862	3.1279	4.5147
K_v (m/s))	0.0105	0.12602	0.12602	0.0105
mass (kg)	1492.38	381.50	338.0	2159.61

results obtained using different $\hat{K}_v$ values for the heuristics and the MILM are reported, allowing the comparison with the solutions of the MINLM given in Table 4. We note that, in this case, adding slenderness constraints does not change the results.

The solutions obtained using the Blackwell's equation[17] for $\hat{K}_v$ (Table 5) present a lower value of the vessel mass than the one obtained by Towler and Sinnot.[6] Also, when a more accurate MINLM (abiding by the dependence of the C_d on the Reynolds number) is used, these solutions are no longer valid and the correct optimal vessels are heavier. This warns that in some cases, the velocity of the vapor is larger than the actual terminal velocity of the droplet associated to the critical diameter, thus implying larger entrainment than assumed. An additional issue emerges observing the result obtained using the MILP with the same $\hat{K}_v$ value as that used by Towler and Sinnot:[6] The discrete nature of the diameters force the choice of a larger diameter (1.5049 m vs 1.25 m). Thus, in practice, a specification of 1.25 m sent to a vessel constructor who is forced to pick standard pipes, will force him to pick 1.5049 m, not 1.25 m and a vessel with 3.75 m instead of 4.5147 m. As a consequence, the H_{vessel}/D_{vessel} ratio falls below the value of 3, which is not recommended.

■ EFFECT OF CRITICAL DROPLET SIZE

The settling velocity v_v depends on the critical droplet diameter, vapor viscosity, the drag coefficient, and the liquid and vapor densities. To explore its influence, we used the MINLM model without H_{vessel}/D_{vessel} constraints to explore the effect of the critical droplet diameter $\hat{d}_{d,\ crit}$ on the final design. The results for different values of $\hat{d}_{d,\ crit}$ are shown in Table 6 and Figure 3, where only the diameter, height, and mass are shown (full results are shown in the Supporting Information). As expected, the utilization of higher critical diameters yielded cheaper vessels, because lower velocities are then allowed, associated to smaller diameters.

■ EFFECT OF LIQUID RESIDENCE TIME

The liquid residence time ($\hat{t}_s$) also has a greater effect on the vessel mass/cost. Cooper et al.[5] recommend 5 to 20 min, although this differs from the recommendations of other

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Table 6. Globally Optimal Results of the MINLM Using Different Values of the Critical Droplet Diameter[a]

	$\hat{d}_{d,\,crit}$ = 75 μm	$\hat{d}_{d,\,crit}$ = 10 μm	$\hat{d}_{d,\,crit}$ = 150 μm	$\hat{d}_{d,\,crit}$ = 200 μm	$\hat{d}_{d,\,crit}$ = 300 μm
D_{vessel} (m)	1.57 / 1.57 / 1.57	1.57 / 1.57 / 1.57	1.57 / 1.57 / 0.84	0.69 / 0.69 / 0.69	0.54 / 0.54 / 0.54
H_{vessel}(m)	2.29 / 2.96/ 2.96	2.29 / 2.96/ 2.96	2.29 / 2.96 / 2.13	2.29/ 2.21 / 2.13	2.46 / 2.39 / 2.31
mass (kg)	478.56 / 562.46 / 562.46	478.56 / 562.46 / 562.46	478.56 / 562.46 / 603.85	495.70 / 483.02 / 470.41	391.43 / 381.50 / 371.63

[a]Results are presented for Couper et al.[5]/Towler and Sinnott[6]/Silla[4]

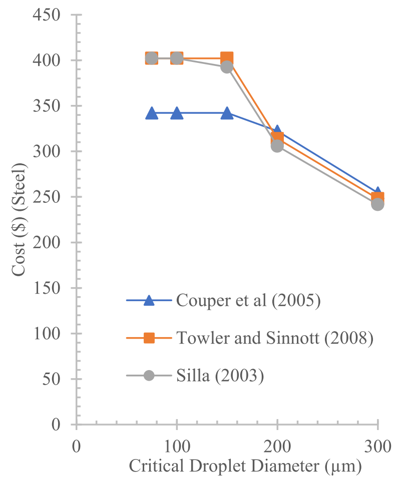

Figure 3. Comparison of the material cost as a function of the critical droplet diameter.

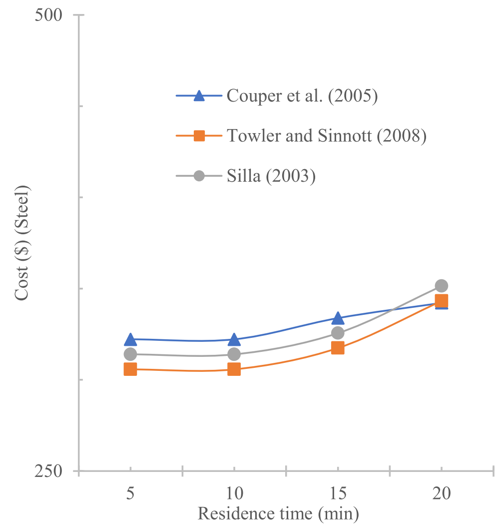

Figure 4. Cost variation as a function of liquid residence time.

authors.[4,6] We think that this parameter could be better determined using some modeling of the level control, and/or the level alarms. However, we explored the values of liquid residence time recommended by Couper et al.[5] We do not impose the height−diameter constraints here. For $\hat{t}_s$ = (5,10,15 and 20) (min) the results are shown in Table 7, where slenderness restrictions are not imposed (full results shown in the Supporting Information). Also, Figure 4 shows the cost as a function of liquid residence time.

Table 7. Globally Optimal Results of the MINLM Using Different Values of Liquid Residence Time[a]

	$\hat{t}_s$ = 5min	$\hat{t}_s$ = 10min	$\hat{t}_s$ = 15min	$\hat{t}_s$ = 20min
D_{vessel} (m)	0.69/ 0.69 / 0.69	0.69/0.69 / 0.69	0.69 / 0.69 / 0.69	1.57 / 0.69 / 0.69
H_{vessel} (m)	2.29 / 2.21/ 2.13	2.29 / 2.21 / 2.13	2.39 / 2.32 / 2.24	2.29 / 2.56 / 2.48
mass (kg)	495.70 / 483.02 / 470.41	495.70 / 483.02 / 470.41	513.63 / 500.96 / 488.35	478.56 / 540.67 / 528.06

[a]Results are presented for Couper et al.[5]/Towler and Sinnott[6]/Silla[4]

The transition from $\hat{t}_s$ = 15 min to $\hat{t}_s$ = 20 min reported in Table 7 using the model present in Couper et al.[5] indicates a reduction of the weight, differently from the trend associated to the other results. This variation occurs because the vessel diameter is higher, but the thickness is lower (3.2 mm), since it reaches the rolled plate diameter. This combination produces lower weight (478.56 vs 513.64 kg). It strikes as puzzling that a vessel with lower wall thickness has actually larger weight, yet it is optimal, but this is easily explained by noting that the cost of plates is different. Simplified design procedures also fail to address these nuances. Also note that the vessel for $\hat{t}_s$ = 20 min, even if has lower weight that the vessel for $\hat{t}_s$ = 15 min, it has higher cost, because we considered higher cost/weight for rolled plates than that for pipes. For more detailed information about the design, see the Supporting Information.

Figure 4 shows that the increase of the residence time demands more expensive vessels, but the magnitude of this increase depends on the features of the separation task.

■ DEMISTER ECONOMIC TRADE-OFF

We selected a horizontal style 4CA pad demister with a $\hat{K}_{v,\,dem}$ of 0.107 from Datta[14] with a density $\hat{\rho}_{demister}$ = 144.2 kg/m^3. The demister height is $\hat{h}_{dem}$ = 0.15 m and its cost is $\hat{C}_{demister}$ = 8.0 US$/kg. In all cases, the height added when a demister is present is different.[4−6] The MINLM was solved using RYSIA without slenderness constraints (H_{vessel}/D_{vessel}). We selected different values of critical droplet diameters ($\hat{d}_{d,\,crit}$) for the comparison (Table 8 and Figure 5). The Supporting Information gives more results.

It can be seen that for the droplet diameter from 75 to 200 μm, the demister renders a lower vessel cost (up to 35.68% for the Silla[4] model and droplet diameters of 75 μm). This analysis is looking strictly at cost. However, if one adds the benefit of reducing vapor entrainment, then demisters are many times desirable regardless of cost.

■ CONSERVATIVE AND OPTIMISTIC MODELS

The above models present a set of options that can be implemented rendering different results. We now present two models, one that picks up the most optimistic and the most pessimistic values. We first note that the options only vary in the choice of vapor and liquid heights. Thus, in eq 46, we choose the minimum $\hat{t}_s$ and the maximum $\hat{t}_s$ for the optimistic and pessimistic models. In turn, the vapor height needs reformulation, instead of eqs 49 through 55, we use the following for the optimistic model:

Table 8. Globally Optimal Results of the MINLM Model with Demister Options[a]

	$\hat{d}_{d,\,crit}$ = 75 μm	$\hat{d}_{d,\,crit}$ = 100 μm	$\hat{d}_{d,\,crit}$ = 150 μm	$\hat{d}_{d,\,crit}$ = 200 μm	$\hat{d}_{d,\,crit}$ = 300 μm
D_{vessel}(m)	0.39 / 0.39 / 0.39	0.39 / 0.39 / 0.39	0.39 / 0.39 / 0.39	0.39 / 0.39 / 0.39	0.39 / 0.54 / 0.54
H_{vessel}(m)	2.90 / 3.53 / 3.51	2.90 / 3.53 / 3.51	2.90 / 3.53 / 3.51	2.90 / 3.53 / 3.51	2.90 / 2.39/ 2.31
mass (kg)	312.07 / 370.92 / 369.16	312.07 / 370.92 / 369.16	312.07 / 370.92 / 369.16	312.07 / 370.92 / 369.16	312.07 / 381.50 / 371.63
demister	yes / yes / yes	yes / yes / yes	yes / yes / yes	yes / yes / yes	yes / no / no

[a]Results are presented for Couper et al.[5]/Towler and Sinnott[6]/Silla[4]

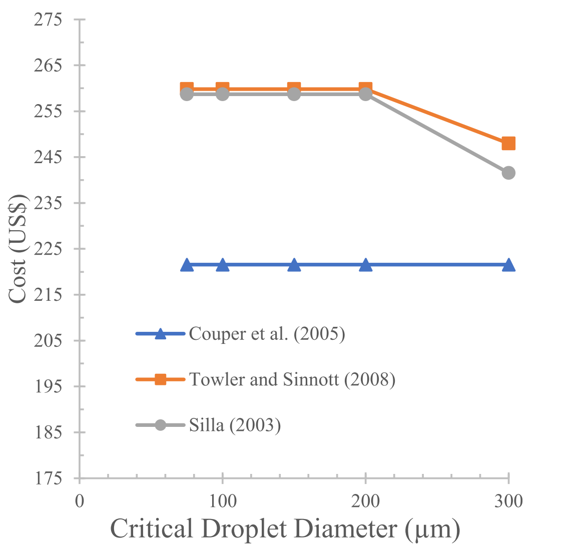

Figure 5. Vessel cost in function of critical droplets diameter—example.

$$H_v = \text{Min}\begin{Bmatrix} 1.6764\,(1-\hat{z}_{dem}) + (1.0668\text{ m} + \hat{d}_{noz} + \hat{h}_{dem})\,\hat{z}_{dem} \\ (H_{inlet-liq} + H_{disengage} + 0.4\,\hat{z}_{dem}) \\ (H_{inlet-liq} + H_{disengage} + 0.4572\hat{z}_{dem}) \end{Bmatrix} \tag{100}$$

$$H_{inlet-liq} \geq \text{Min}\{\text{Max}\{0.5D_{vessel},\, 0.6\text{ m}\},\, \text{Max}\{0.5D_{vessel},\, 0.6096\text{ m}\}\} \tag{101}$$

$$H_{disengage} \geq \text{Min}\{\text{Max}\{D_{vessel},\, 1\text{ m}\},\, \text{Max}\{D_{vessel},\, 0.9144\text{ m}\}\} \tag{102}$$

where $\hat{d}_{noz}$ here is taken as the smaller diameter (obtained using $\hat{u}_n(\text{ft}/s) = 100\sqrt{\hat{\rho}_{mix}}$).

Equation 100 is linearized as follows:

$$H_v \leq 1.6764\,(1 - z_{dem}) + (1.0668\text{ m} + \hat{d}_{noz} + \hat{h}_{dem})z_{dem} + \hat{\Gamma}\,yv_1 \tag{103}$$

$$H_v \leq (H_{inlet-liq} + H_{disengage} + 0.4\,z_{dem}) + \hat{\Gamma}\,yv_2 \tag{104}$$

$$H_v \leq (H_{inlet-liq} + H_{disengage} + 0.4572\,z_{dem}) + \hat{\Gamma}\,yv_3 \tag{105}$$

$$H_v \geq 1.67585\,(1 - \hat{z}_{dem}) + (1.0668\text{ m} + \hat{d}_{noz} + \hat{h}_{dem})\,z_{dem} - \hat{\Gamma}\,yv_1 \tag{106}$$

$$H_v \geq (H_{inlet-liq} + H_{disengage} + 0.4\,z_{dem}) - \hat{\Gamma}\,yv_2 \tag{107}$$

$$H_v \geq (H_{inlet-liq} + H_{disengage} + 0.4572\,z_{dem}) - \hat{\Gamma}\,yv_3 \tag{108}$$

$$yv_1 + yv_2 + yv_3 = 1 \tag{109}$$

Indeed if, for example, $yv_1 = 0$, eqs 104 and 107 identify $1.6764\,(1 - z_{dem}) + (1.0668\text{ m} + \hat{d}_{noz} + \hat{h}_{dem})z_{dem}$ as the minimum, all the other equations becoming trivial.

Equation 101 can be rewritten as follows:

$$H_{inlet-liq} \geq 0.6\text{ m} \tag{110}$$

$$H_{inlet-liq} \geq 0.5D_{vessel} \tag{111}$$

Finally, eq 102 is linearized as follows:

$$H_{disengage} \geq D_{vessel} \tag{112}$$

$$H_{disengage} \geq 0.9144\text{ m} \tag{113}$$

The maximum operators written in this simplified form will render binding equations because the objective function will force it.

In turn, the pessimistic model uses the following equations:

$$H_v = \text{Max}\begin{Bmatrix} 1.6764\,(1 - z_{dem}) + (1.0668\text{ m} + \hat{d}_{noz} + \hat{H}_{dem})z_{dem} \\ (H_{inlet-liq} + H_{disengage} + 0.4\,z_{dem}) \\ (H_{inlet-liq} + H_{disengage} + 0.4572\,z_{dem}) \end{Bmatrix} \tag{114}$$

$$H_{inlet-liq} \geq \text{Max}\{\text{Max}\{0.5D_{vessel},\, 0.6\text{ m}\},\, \text{Max}\{0.5D_{vessel},\, 0.6096\text{ m}\}\} \tag{115}$$

$$H_{inlet-liq} \geq \text{Max}\{\text{Max}\{0.5D_{vessel},\, 0.6\text{ m}\},\, \text{Max}\{0.5D_{vessel},\, 0.6096\text{ m}\}\} \tag{116}$$

where $\hat{d}_{noz}$ is taken as the larger diameter, that is, using $\hat{u}_n(\text{ft}/s) = 60\sqrt{\hat{\rho}_{mix}}$..

Equations 106–108are represented by:

$$H_v \geq 1.6764\,(1 - \hat{z}_{dem}) + (1.0668 + \hat{d}_{noz} + \hat{h}_{dem})z_{dem} \tag{117}$$

$$H_v \geq (H_{inlet-liq} + H_{disengage} + 0.4\,z_{dem}) \tag{118}$$

$$H_v \geq (H_{inlet-liq} + H_{disengage} + 0.4572\,z_{dem}) \tag{119}$$

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$$H_{\text{inlet-liq}} \geq 0.5D_{\text{vessel}} \quad (120)$$

$$H_{\text{inlet-liq}} \geq 0.6096 \quad (121)$$

$$H_{\text{disengage}} \geq D_{\text{vessel}} \quad (122)$$

$$H_{\text{disengage}} \geq 1 \quad (123)$$

In Table 9 and Figure 6, we compare the optimistic and pessimistic results including the choice of the demister for different critical droplet diameters. We note that, in the case where a demister is used, it makes no sense reporting the value of $d_{\text{d, eff}}$.

Table 9. Results of Optimistic/Pessimistic (MINLM)

	$\hat{d}_{\text{d, crit}}$ = 75 μm	$\hat{d}_{\text{d, crit}}$ = 100 μm	$\hat{d}_{\text{d, crit}}$ = 150 μm	$\hat{d}_{\text{d, crit}}$ = 200 μm	$\hat{d}_{\text{d, crit}}$ = 300 μm
D_{vessel}(m)	0.39/0.39	0.39/0.39	0.39/0.39	0.39/0.39	0.39 0.54
H_{vessel}(m)	2.13/5.12	2.13/5.12	2.13/5.12	2.13/5.12	2.13/3.25
mass(kg)	239/521	239./521	239/521	239/521	239/494
demister	yes / yes	yes / yes	yes / yes	yes / yes	yes / no

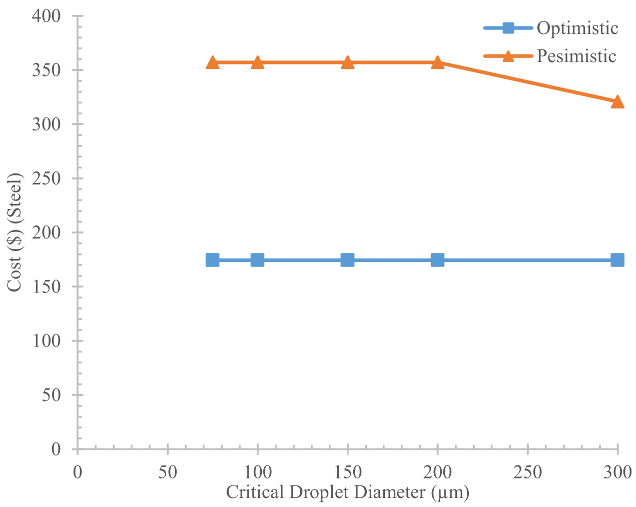

Figure 6. Results of optimistic/pessimistic (MINLP model).

The MINLM results from previous sections can be allocated between the values from optimistic and pessimistic results of this section. The comparison between the optimistic and pessimistic results displayed in Figure 6 shows that there is a considerable gap among the alternative designs obtained through different heuristics. The Supporting Information shows additional results.

CONCLUSIONS

We developed an MINLP model that can identify the least-cost design automatically, without the need of direct interference of the designer.

The analysis of design results based on fixed $\hat{K}_v$ values (without demister), using heuristics or a linear model, showed that the nonlinear approach that consider the dependence of the C_D with the Reynolds number provides much different results, thus calling for the abandoning of the use of heuristics as well as the MILM. In addition, we highlighted the importance of using discrete values of diameters and plates as opposed to considering them continuous, rounding them up to the next second decimal, which leads to other problems.

Because of different criteria existing for selecting the height of the vessel, we also built and analyzed optimistic and pessimistic models. In addition, we explored the impact of some design parameters as well as the use of demisters.

The set of results indicates that the proposed approach can be a useful task for design staffs, thus allowing the reduction of capital costs and engineering work force associated to the design of separation vessels.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.0c04379.

Additional analysis of the effect of critical droplet size, liquid residence time, demister economic tradeoff, conservative and optimistic models, and comparison of results from heuristics (PDF)

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Notes

The authors declare no competing financial interest.

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NOMENCLATURE

Sets

prop Pipe property
s Velocity partition
std Nominal pipe diameter

Parameters

$\hat{C}_{\text{steel}}$ Steel cost (US$/kg)
$\hat{C}_{\text{steel, std}}$ Steel cost (US$/kg) over the set of pipes or rolled plates.
$\hat{C}_{\text{demister}}$ Demister cost (US$/kg)

$\hat{D}_{d}$ Droplet diameter (m)
$\hat{d}_{d,\ crit}$ Droplet critical diameter (m)
$\hat{D}_{min}$ Minimal vessel diameter (m)
$\hat{d}_{noz}$ Inlet nozzle diameter
$\hat{E}$ Joint efficiency
$\hat{h}_{dem}$ Demister height (m)
$\hat{K}_{v}$ Vapor constant coefficient (m/s)
$\hat{K}_{v,\ dem}$ Vapor constant coefficient for demister (m/s)
$\hat{\mu}$ Dynamic viscosity (Pa·s)
$\hat{\rho}_{l}$ Liquid density (kg/m^3)
$\hat{\rho}_{v}$ Vapor density (kg/m^3)
$\hat{\rho}_{steel}$ Density of the material used in the vessel construction (steel density) (kg/m^3)
$\hat{\rho}_{dem}$ Demister density (kg/m^3)
$\hat{\rho}_{mix}$ Mixed density (lb/ft^3)
$\hat{P}$ Maximum operating pressure difference (psig)
$\hat{Q}_{l}$ Liquid flow rate (m^3/s)
$\hat{Q}_{v}$ Vapor flow rate (m^3/s)
$\hat{\Gamma}$ Constant for decomposition
$\hat{\Gamma}_{h}$ Constant for linearization of $yvessel_{std}\ H_{vessel}$
$\hat{\Gamma}_{w}$ Constant for linearization of $yvessel_{std}$·Mass
$\hat{S}$ Allowable tensile stresses (psi)
$\hat{t}_{min}$ Minimum wall thickness (mm)
$\hat{t}_{s}$ Surge time liquid (or residence time) (seconds)
$\hat{u}_{n}$ Inlet nozzle velocity
$\hat{V}_{v\_const}$ Vapor velocity constant (m/s)
$\hat{V}_{demister}$ Demister volume (m^3)
$\widehat{Vessel}_{std,\ int\ d}$ Inner diameter intd of vessel option std
$\widehat{Vessel}_{std,\ t_{shell}}$ Shell thickness t_{shell} of vessel option std
$\widehat{Vessel}_{std,\ th}$ Head thickness t_{shell} of vessel option std
$\hat{vs}_{s}(s)$ Value of velocity in partition (m/s)

Binary Variables

$yvessel_{std}$ Binary variable to denote a pipe selection
yvs_{s} Binary variable to denote a selection of velocity interval
$wvesszhh_{std,\ hh}$ Binary variable to denote a $yvessel_{std}\ z_{hh}$
$wvesszhe_{std,\ he}$ Binary variable to denote a $yvessel_{std}\ z_{he}$
z_{he} Binary variable to denote a selection of ellipsoidal head
z_{hh} Binary variable to denote a selection of hemispherical head
z_{dem} Binary variable to denote a selection of demister
$w_{dem}vessel_{std}$ Binary variable to denote a $yvessel_{std}\ z_{dem}$

Variables

C_{d} Drag coefficient
C_{vessel} Total vessel cost (US$)
D_{vessel} Vessel diameter (m)
$H_{disengage}$ Disengage height (m)
$H_{inlet-liq}$ Inlet liquid height (m)
H_{l} Liquid height (m)
H_{v} Vapor height (m)
H_{vessel} Vessel height (m)
Mass Vessel mass (kg)
R_{e} Reynolds number
t_{h} Head thickness (m)
t_{shell} Shell thickness (m)
v_{v} Terminal vapor velocity (m/s)
$v_{v,\ C}$ Terminal vapor velocity (m/s) in function of C_{d}
$v_{v,\ real}$ Real vapor velocity (m/s)
V_{head} Head volume (m^3)
V_{shell} Shell volume (m^3)
$whvessel_{std}$ Variable to denote the product $yvessel_{std}H_{vessel}$
$wvel_{dem}$ Variable to denote the product $v_{v,\ C}z_{dem}$
$wvol_{dem}$ Variable to denote the product $V_{dem}z_{dem}$
$wmass_{std}$ Variable to denote the product $yvessel_{std}$mass

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