A COMPARISON OF STRATEGIES FOR OPTIMIZATION OF COMPLEX DISTILLATION COLUMNS

Filipe J.M. Neves and Nuno M.C. Oliveira*
GEPSI - PSE Group, Department of Chemical Engineering, University of Coimbra
Pólo II, Pinhal de Marrocos, 3030-290 Coimbra, Portugal

Abstract

This work compares several strategies developed for the economical optimization of large-scale complex distillation columns. The performance of each strategy is illustrated considering two examples drawn from industry, regarding the aniline production by liquid hydrogenation of nitrobenzene. Since discrete decisions are involved, related to the optimal location of feed streams and the total number of equilibrium stages, we consider both the classical MINLP approach (Viswanathan and Grossman, 1993) as well as two recently continuous NLP approaches (Lang and Biegler, 2002; Neves et al., 2003). The results obtained show that all strategies are capable of converging to the best optimal solution that it was possible to found, with proper pre-processing, and when a suitable numerical solver is selected.

Keywords

Distillation columns, Optimization, MINLP, Continuous approaches.

Introduction

Although more general, and perhaps more intuitive and easier to develop, discrete models for the optimization of complex distillation columns are frequently encumbered by numerical difficulties faced by current codes for solution of MINLP problems, such as DICOPT. This can happen during either the solution of the NLP subproblems, or during the MILP phase, due to high nonconvexity of the problem, that prevents the generation of valid lower bounds (Barttfeld et al., 2003).

A strategy based on continuous optimization was recently proposed by Lang and Biegler (2002). The main idea is to use a distribution function (DDF), characterized by a dispersion factor σ around a central value that will be optimized, in order to select the appropriate location for a given stream. This approach often requires the use of different values of σ within the same problem, to avoid premature convergence to local optima. During the early solution phases, a sufficiently large value of the parameter σ is considered, producing a wide distribution that covers significantly all of the candidate trays. Thus, the stream is initially distributed to the most favorable region in the column. As the solution proceeds, smaller values of σ are progressively introduced, leading to narrower distributions, and therefore to the iterative optimal location of the stream.

An alternative formulation, also based on the use of only continuous variables was introduced by Neves et al. (2003). Initially, the feed and product streams are distributed to each tray of the column, using continuous variables $b_{i,j}$. These variables represent the split fraction of a given stream k (feed or product) among the different equilibrium stages j of the column, and thus satisfy the conservation equations

$$\sum_{j}^{np} b_{kj} = 1, \qquad k \in S.$$

By imposing simple concave constraints of the form

$$\sum_{j}^{np} b_{kj}^2 \geq \alpha_k, \qquad k \in S$$

with an adjustable parameter $\alpha_k \in [0,1]$, the best location of each stream can also be determined. This corresponds to single equilibrium stages, when $\alpha \to 1$, and to preferable regions, with $\alpha < 1$. Unlike the use of distribution functions, these regions do not need to be continuous.

* To whom all correspondence should be addressed. Email: nuno@eq.uc.pt.

MESH equations

Summation:

$$\sum_{i}^{nc} x_{ij} = 1 \text{ and } \sum_{i}^{nc} y_{ij} = 1, \quad j = 1,\ldots,np \qquad (4)$$

Equilibrium:

$$y_{i,j} = K_{i,j} x_{i,j} - \varepsilon EQ_{i,j} \quad i = 1,..,nc \quad j = 1,..,np \qquad (5)$$

Properties Correlations

$$HL_j = f\left(x_{i,j}, T_j\right) \qquad (1)$$

$$HV_j = f\left(y_{i,j}, T_j\right) \qquad (2)$$

$$K_{i,j} = f\left(x_{i,j}, T_j\right) \text{ (UNIFAC model)} \qquad (3)$$

Mass & energy balances

Condenser (j=1 ; i=1,…,nco):

$$V_{j+1} = L_j \left(1 + 1/RR\right) - \varepsilon BMT_j \qquad (6)$$

$$V_{j+1} y_{i,j+1} = L_j \left(1 + 1/RR\right) x_{i,j} - \varepsilon BMP_{i,j} \qquad (7)$$

$$Q_C + V_{j+1} HV_{j+1} = L_j \left(1 + 1/RR\right) HL_j - \varepsilon BE_j \qquad (8)$$

Column (j=2,…,np-1 ; i=1,…,nco):

$$L_{j-1} + V_{j+1} + F_0 b_{F,j} + RR\, D\, b_{C,j} + V_{np} b_{R,j} = \left(L_j + U_0 b_{LS,j} + V_j + W_j\right) - \varepsilon BMT_j \qquad (9)$$

$$L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} + F_0 b_{F,j} x_{i,F} + RR\,D\, b_{C,j} x_{i,1} + V_{np} b_{R,j} y_{i,np} = \left(L_j + U_0 b_{LS,j}\right) x_{i,j} + \left(V_j + W_0 b_{VS,j}\right) y_{i,j} - \varepsilon BMP_{i,j} \qquad (10)$$

$$L_{j-1} HL_{j-1} + V_{j+1} HV_{j+1} + F_0 b_{F,j} HF + RR\,D\, b_{C,j} HL_1 + V_{np} b_{R,j} HV_{np} = \left(L_j + U_0 b_{LS,j}\right) HL_j + \left(V_j + W_0 b_{VS,j}\right) HV_j - \varepsilon BE_j \qquad (11)$$

Reboiler (j=np ; i=1,…,nco):

$$L_{j-1} = L_j + V_j - \varepsilon BMT_j \qquad (12)$$

$$L_{j-1} x_{i,j-1} = L_j x_{i,j} + V_j y_{i,j} - \varepsilon BMP_{i,j} \qquad (13)$$

$$Q_R + L_{j-1} HL_{j-1} = L_j HL_j + V_j HV_j - \varepsilon BE_j \qquad (14)$$

Cost Expressions

Fixed column costs (shell and internals)

$$d = f\left(V_j, T_j\right) \text{ and } h = f\left(b_{C,j}, b_{R,j}\right) \qquad (15)$$

$$C_{SI} = f(d, h) \qquad (16)$$

Fixed exchanger costs (Cond./Reboiler)

$$A_C = f\left(T_1, Q_C\right) \text{ and } A_R = f\left(T_{np}, Q_R\right) \qquad (17)$$

$$C_{CR} = f\left(A_C, A_R\right) \qquad (18)$$

Operational heat exchanger costs

$$C_{CU} = f\left(Q_C\right) \text{ and } C_{HU} = f\left(Q_R, T_{np}\right) \qquad (19)$$

$$C_U = C_{CU} + C_{HU} \qquad (20)$$

Total costs

$$C_T = C_{SI} + C_{CR} + C_U \qquad (21)$$

Convergence Expressions

(applicable only in the DDF based strategy)

Feed and product stream convergence:

$$b_{LS,j} = \exp\left(-\left((j - nls)/\sigma\right)^2\right) / \sum_k \exp\left(-\left((k - nls)/\sigma\right)^2\right),$$

$$b_{VS,j} = \exp\left(-\left((j - nvs)/\sigma\right)^2\right) / \sum_k \exp\left(-\left((k - nvs)/\sigma\right)^2\right),$$

$$b_{F,j} = \exp\left(-\left((j - nf)/\sigma\right)^2\right) / \sum_k \exp\left(-\left((k - nf)/\sigma\right)^2\right),$$

$$b_{C,j} = \exp\left(-\left((j - nc)/\sigma\right)^2\right) / \sum_k \exp\left(-\left((k - nc)/\sigma\right)^2\right),$$

$$b_{R,j} = \exp\left(-\left((j - nr)/\sigma\right)^2\right) / \sum_k \exp\left(-\left((k - nr)/\sigma\right)^2\right) \qquad (24)$$

(applicable with the split fraction based strategy)

Feed and product stream convergence:

$$\sum_{j=1}^{np} b_{F,j}^2 \geq \alpha_F, \quad \sum_{j=1}^{np} b_{C,j}^2 \geq \alpha_C, \quad \sum_{j=1}^{np} b_{R,j}^2 \geq \alpha_R,$$

$$\sum_{j=1}^{np} b_{LS,j}^2 \geq \alpha_{LS} \text{ and } \sum_{j=1}^{np} b_{VS,j}^2 \geq \alpha_{VS} \qquad (25)$$

(applicable only in the MINLP based strategy)

Feed and product stream convergence:

$$b_{F,j},\ b_{C,j},\ b_{R,j},\ b_{LS,j},\ b_{VS,j} \text{ as BINARY VARIABLES} \qquad (26)$$

Auxiliary Expressions

Split fractions control:

$$\sum_{j=1}^{np} b_{F,j} = 1, \sum_{j=1}^{np} b_{C,j} = 1, \sum_{j=1}^{np} b_{R,j} = 1, \sum_{j=1}^{np} b_{R,j} = 1, \sum_{j=1}^{np} b_{R,j} = 1 \qquad (22)$$

Slack constraints:

$$\left\|\varepsilon BMT_j\right\| \leq \delta, \quad \left\|\varepsilon BMP_{i,j}\right\| \leq \delta, \quad \left\|\varepsilon EQ_{i,j}\right\| \leq \delta,$$

$$\left\|\varepsilon BE_j\right\| \leq \delta \qquad (23)$$

Formulation

$$\min_{b_{F,j}, b_{C,j}, b_{R,j}, b_{LS,j}, b_{VS,j}, RR} C_T \qquad (27)$$

$$s.t. \quad (1) - (23)$$

DDF based: add equations (24)
Fraction based: add equations (25)
MINLP based: declare variables as in (26)

Figure 1 – Formulation for the optimization of a distillation unit, using three different strategies (DDF, split fraction and MINLP based).

This allows the determination of optimal locations for complex columns with split feed or product streams, and the tradeoffs between multiple and single locations to be observed in an objective function. Similarly to the DDF approach, this strategy can also be sensitive to the presence of local optima. Thus a relaxed solution for the optimization problem, with α_k=0, is initially obtained. This solution is later refined by solving the optimization problem with increasing values of α_k.

Formulation

Figure 1 presents the complete formulation for the economical optimization of a distillation unit, using the three strategies in study, for a column with a total condenser and a partial reboiler. In these expressions, *np* and *nco* represent the number of plates and the number of components; *nf*, *nc*, *nr* the location of the feed, reflux and reboil streams; *nls* and *nvs* the location of liquid and vapor side-streams; L_j and V_j the liquid and vapor flows; T_j the temperature profile; HL_j and HV_j the liquid and vapor enthalpies; K_{ij} the liquid-vapor equilibrium constant; x_{ij} and y_{ij} the liquid and vapor compositions; F_0 and $x_{i,F}$ the feed flowrate and composition; *RR* the reflux ratio; U_0 and W_0 the liquid and vapor side-stream flows; *d* and *h* the diameter and height of the column; A_C , A_R , Q_C and Q_R the areas and heats regarding the condenser and reboiler; $\varepsilon EQ_{i,j}$, $\varepsilon BMP_{i,j}$, εBMT_j and εBE_j the slack variables relative to the equilibrium, mass (partial and total) and energy balance equations; $b_{F,j}$, $b_{C,j}$, $b_{R,j}$,$b_{LS,j}$ and $b_{VS,j}$ the fraction variables associated to the feed, product (top and bottom) and side-streams (liquid and vapor); α_F, α_C, α_R, α_{LS} and α_{VS} the adjustable parameters concerning the same streams previously enumerated; δ the tolerance; C_{SI}, C_{CR} the fixed column cost (shell and internals) and fixed exchanger cost (reboiler and condenser); C_{CU}, C_{HU}, C_U the cold, hot and total utility cost; C_T the total cost (objective function).

A key aspect for the successful application of all strategies consists in the robust initialization, scaling and bounding of the problem variables and equations, in a pre-processing phase, that uses a combination of shortcut methods (to determine the maximum allowed number of plates and the respective minimum required reflux ratio) and a self-initialized iterative method for a previous solution of the distillation models. Slack variables are added to the main MESH equations to allow a faster solution start, avoiding problems caused by infeasibilities. Maintaining bounds for the maximum magnitude of these variables corresponds to defining a region where the problem is solved, within a certain tolerance. For the purpose of initialization this admissible error reduces, in a very significant manner, the required computation time.

Main results

In the first example, the objective was to synthesise a column that could recover, in the bottom, aniline and nitrobenzene. The feed was contaminated with cyclo-hexilamine for which a maximum allowed molar fraction in the bottom was set. This problem involved the solution of a model with approximately 6500 equations and variables, for a maximum allowed number of plates equal to 50.

Table 1 – Results obtained for example 1; (a) based on split fractions, (b) MINLP based, (c) common to both strategies.

	Pre-processing Phase	Optimization Phase	
		Relaxed	Integer
RR	2.370 (c)	2.961 (c)	3.008 (a) / 2.925 (b)
$b_{C,j}$	$b_{C,2} \ldots b_{C,21} = 0.05$ (a) / $b_{C,2} = 1$ (b)	$b_{C,18} = 0.475$, $b_{C,19} = 0.525$ (c)	$b_{C,19} = 1$ (a) / $b_{C,18} = 1$ (b)
$b_{F,j}$	$b_{F,40} \ldots b_{F,49} = 0.1$ (a) / $b_{F,44} = 1$ (b)	$b_{F,46} = 1$ (c)	$b_{F,46} = 1$ (c)
$b_{R,j}$	$b_{R,49} = 1$ (c) (FIXED)	$b_{R,49} = 1$ (c) (FIXED)	$b_{R,49} = 1$ (c) (FIXED)
C_T (€/year)	N.A.	382 589 (c)	382 966 (a) / 382 962 (b)
Time (s)	20 (a) / 20 (b)	5 (a) / 11 (b)	4 (a) / 5 (b)

Table 2 – Results for example 1, using the DDF strategy.

	Pre-processing Phase	Optimization Phase		
		$\sigma = 0.9$	$\sigma = 0.35$	$\sigma = 0.10$
RR	2.370	2.967	2.896	2.925
$b_{C,j}$	In accordance: NC = 10, $\sigma_C = 0.9$	NC = 18.479, $b_{C,17} = 0.042$, $b_{C,18} = 0.473$, $b_{C,19} = 0.448$, $b_{C,20} = 0.036$	NC = 17.549, $b_{C,17} = 0.311$, $b_{C,18} = 0.689$	NC=17.960, $b_{C,18} = 1$
$b_{F,j}$	In accordance: NF = 44, $\sigma_F = 0.9$	NF = 46.123, $b_{F,45} = 0.132$, $b_{F,46} = 0.615$, $b_{F,47} = 0.242$, $b_{F,48} = 0.008$	NF = 46.018, $b_{F,46} = 0.999$	NF=41.010, $b_{F,46} = 1$
$b_{R,j}$	$b_{R,49} = 1$ (FIXED)	$b_{R,49} = 1$ (FIXED)	$b_{R,49} = 1$ (FIXED)	$b_{R,49} = 1$ (FIXED)
C_T (€/year)	N.A.	383 053	382 758	382 962
Time (s)	20	28	15	16

These results refer to a variable feed (candidate trays: 40…49) using a variable reflux (candidate trays: 2…21) approach with fixed reboiler. For the strategy based on split fractions, the optimization problem was initiated with the reflux stream equally divided among the candidate trays. The MINLP strategy was initialized with the integer solution obtained by application of a shortcut method, with all streams entering in single locations. Slightly different solutions were obtained using the MINLP and split fraction strategies, due to the similar value of C_T in the two configurations obtained (within the numerical tolerance imposed).

In the second example, the objective was to synthesise a column that could separate aniline plus four "heavy" components (cyclohexylidenoaniline, dicyclohexylamine fenylcyclohexylamine and nitrobenzene) from a contaminated feed with 5 light parasite components (benzene, water, cyclohexylamine, cyclohexanone and cyclohexanol). The operational specification concerned the maximum molar fraction of cyclo-hexylamine allowed in the bottom. This problem involved the solution of models with approximately 18000 equations and variables, and a maximum allowed number of plates equal to 30.

Table 3 – Results for example 2, using the MINLP strategy.

	Pre-processing Phase	Optimization Phase	
		Relaxed	Integer
RR	0.0453	0.0569	0.0580
$b_{C,j}$	$b_{C,2} = 1$ (FIXED)	$b_{C,2} = 1$ (FIXED)	$b_{C,2} = 1$ (FIXED)
$b_{F,j}$	$b_{F,2}\ldots b_{F,6} = 0.2$	$b_{F,4} = 1$	$b_{F,4} = 1$
$b_{R,j}$	$b_{R,10}\ldots b_{R,29} = 0.05$	$b_{R,18} = 0.722$; $b_{R,19} = 0.278$	$b_{R,18} = 1$
C_T (€/year)	N.A.	187 137	187 244
Time (s)	227	238	329

Table 4 – Results for example 2, using the split fraction based strategy.

	Optimization Phase			
	Relaxed	Integer		
		$\delta=1\text{x}10^{-5}$	$\delta=5\text{x}10^{-6}$	$\delta=1\text{x}10^{-6}$
RR	0.0453	0.0552	0.0567	0.0580
$b_{C,j}$	$b_{C,2} = 1$ (FIXED)	$b_{C,2} = 1$ (FIXED)		
$b_{F,j}$	$b_{F,4} = 1$	$b_{F,4} = 1$		
$b_{R,j}$	$b_{R,18} = 0.722$; $b_{R,19} = 0.278$	$b_{R,18} = 1$		
C_T (€/year)	187 137	186 976	187 125	187 244
Time (s)	225	106	46	51

Table 5 – Results for example 2, using the DDF strategy.

	Pre-Processing Phase	Optimization Phase		
		($\sigma = 0.9$)	($\sigma = 0.35$)	($\sigma = 0.10$)
RR	0.0453	0.0639	0.0571	0.0580
$b_{C,i}$	$b_{C,2} = 1$ (FIXED)	$b_{C,2} = 1$ (FIXED)	$b_{C,2} = 1$ (FIXED)	$b_{C,2} = 1$ (FIXED)
$b_{F,i}$	In accordance: NF = 4 $\sigma_F = 0.9$	NF = 4.796 $b_{F,3} = 0.012$; $b_{F,4} = 0.287$; $b_{F,5} = 0.595$; $b_{F,6} = 0.105$;	NF = 4.11 $b_{F,4} = 0.998$	NF=4 $b_{F,4} = 1$
$b_{R,i}$	In accordance: NR = 20 $\sigma_R = 0.9$	NR = 18.493 $b_{R,17} = 0.040$; $b_{R,18} = 0.465$; $b_{R,19} = 0.457$; $b_{R,20} = 0.038$;	NR = 17.57 $b_{R,17} = 0.241$ $b_{R,18} = 0.759$	NR=18 $b_{R,18} = 1$
C_T (€/year)	N.A.	187 880	187 242	187 244
Time (s)	245	161	347+170	87

For the example 2, the reported results refer to a variable feed (candidate trays: 2…6) and variable reboil (candidate trays: 10…29) approach, the most efficient approach for the column in study. In the pre-processing phase, the streams were splitted equally among the candidate trays, even when using the MINLP strategy, because this proved to be necessary for the solution of the RMINLP problem.

In the strategy based on split fractions, 3 values of δ were used due to the large dimension/complexity of the problem. The main idea is to solve the optimization problem in sequential steps, where the value of tolerance is successively decreased until all the MESH equations are verified within a negligible error – this will prevent large numbers of infeasibilities and avoid solver failures.

The reported CPU times for the DDF strategy, have 2 components for each value of σ, because the high complexity of the problem requires a new pre-processing phase each time the value of the dispersion factor is decreased – not doing this resulted in solver failures.

For all of the results presented, a 2.6 GHz Pentium IV computer and the modelling environment GAMS were used. MINOS, SNOPT and CONOPT III were tested as continuous solvers. Only CONOPT III was capable of converging the continuous strategies. Regarding the MINLP strategy, the DICOPT++ solver failed with both examples (using default numerical parameters). The solution of the MINLP problems was obtained with the SBB solver.

Conclusions

The results obtained were confirmed, using detailed calculations; this requires identifying for each *np*, the best location for the feed stream and the reflux ratio that allows the minimization of the objective function (a time-consuming study due to the required number of discrete runs). In general, all strategies were capable of converging to the best optimal solution that it was possible to found, when proper pre-processing care is taken, and when a suitable numerical solver is selected. The computation times obtained are within the same order of magnitude.

References

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

Lang,Y-D, Biegler, L.T. (2002). A Distributed Stream Method for Tray Optimization. *AIChE Journal, 48*, 582.

Neves, F.J.M., Silva, D.C.M., Oliveira, N.M.C. (2003). A Robust Strategy for Optimizing Complex Distillation Columns. *Accepted in Escape-14 - European Symposium on Computer Aided Process Engineering*, Lisbon.

Viswanathan, J., Grossman, I. E. (1993). An alternate MINLP model for finding the number of trays required for a specified separation objective. *Computers and Chemical Engineering 17*, 949.