Evaluation of Design Flexibility in Distillation Columns Using Rigorous Models

Patricia M. Hoch, Ana M. Eliceche, Ignacio Grossman

EDRC 06-187-95

EVALUATION OF DESIGN FLEXIBILITY IN DISTILLATION COLUMNS USING RIGOROUS MODELS

Patricia M. Hoch\ Ana M Ebceche* and Ipiaao E. Grossmann#

+ PLAPIQUI - Univeradad Nacional del Sur-12 dcOctubrc 1S42 - S000 Bahia Blanca - ARGENTINA
*Chem. Eog, Dept. Carnegie Mellon University, Pittsburgh, Pennsylvania 15213 - USA

ABSTRACT

A methodology is presented for the evaluation of the flexibility and bottlenecks detection of a given distillation column design, using rigorous simulation models. The flexibility index is calculated as proposed by Swaney and Grossmann (1985), solving a nonlinear programming (NLP) problem in the direction of each vertex in the uncertain space, in which the objective is die maximization of the displacements. The control variables, reflux and product flow rates, are the optimization variables of the NLP. The purity specifications, recovery and maximum equipment capacities are posed as the constraints for feasibility of the NLP. Numerical results will be presented for the case of a debutanizer column. Uncertainties are considered in components feed flow rate, maximum allowed vapor velocity, heat transfer coefficients of condenser and reboiler, and cooling water inlet temperature. Great physical insight can be gained from the NLP solutions in the directions of the vertices, detecting bottlenecks and the worst combinations of uncertain parameters.

KEYWORDS

Distillation columns, design, flexibility, bottlenecks.

INTRODUCTION

The design of distillation columns with nominal parameters has been extensively studied in the literature. Recently, the design of distillation columns with uncertain parameters has been addressed. Fisher *et a!.* (1985) studied the effect of overdesign in die operability of distillation columns when changes in the feed composition are expected. Kubic and Stein (1988) considered random and fuzzy uncertainties in the design of distillation columns.

Flexibility analysis in the design of chemical processes has also received increasing attention in the literature. Swaney and Grossmann (1985) presented an index for operational flexibility. A recent updated review of techniques for flexibility can be found in Grossmann and Straub (1991).

Hoch and Hiceche (1994) considered the design of distillation columns with uncertainties in the feed, model and cost parameters. At the design stage, the objective was to size the column so that in the uncertain space considered a feasible operation would be achieved. The contribution of each uncertain parameter to each size is quantified, so the error of using a subset of parameters can be estimated.

The purpose of this work is to calculate the flexibility and predict equipment bottlenecks in the presence of uncertain parameters for a given column design. The combination of uncertain parameters in which the bottlenecks will occur is also detected.

FLEXIBILITY EVALUATION

There are two types of analysis for design flexibility:

1- Feasibility test, which evaluates the feasibility of a design for a given range of disturbances:

where 6 is a vector of dimension N* which contains the uncertain parameters, and the upper and lower bounds are fixed.

2- Flexibility index, defined by Swaney and Grossmann, (1985). The objective here is to find a measure of how flexible Ae design is, defining a maximum range of values for the uncertain parameters. Inside these bounds, feasible operation is achieved. They are defined as:

$$e^N - FAS-* e * e^N + FAO* \qquad (2)$$

where 8^N is the nominal value for the uncertain parameters, A8+ and AO" being die positive and negative expected deviations, and F is *the flexibility index* (Swaney y Grossmann, 1985).

The behavior of a given process can be represented by the set of equations:

$$\begin{aligned} k(d,z,x,9) &= 0 \\ g(d,z,x,\theta) &\leq 0 \end{aligned} \qquad (3)$$

where h are the set of equations representing the steady state of the column, and g is the set of design constraints which must be fulfilled for a feasible operation.

The variables can be classified as:

- d: design variables, which define the process structure and equipment size, fixed at the design stage,
- 6: uncertain parameters,
- z: control variables (degrees of freedom),
- x: state variables

Once d is selected, for any realization of 6, state variables can be expressed as an implicit function of the variables z, solving h=O:

$$h(d,z,x,\theta) = 0 \Rightarrow x = x(d,z,\theta) \qquad (4)$$

State variables can be eliminated and the process can be described with the set of inequalities.

$$g_j[d,z,x(d,z,\theta),\theta] = f_j(d,z,\theta) \quad j \in J \qquad (5)$$

where j is the index of the inequality constraints. The value of f determines the feasibility or unfeasibility of a design. As z can be adjusted such that (5) is satisfied, then die feasibility for a given d,6 means that z exists which satisfies (5).

Given the nominal values 6^N and their expected deviations, there will be a set T of uncertain parameters:

$$T = \{\theta / \theta^{Low} \leq \theta \leq \theta^{Upp}\} \qquad (6)$$

where lower and upper bounds are calculated as Q^{1}" - 6^N - A6~, d^{Vwf} « 6^N + A6* respectively.

As 6^N leads to a feasible design, F can be defined as the maximum deviation 6 applicable to each one of die expected deviations AO",A6* such that the design is still feasible.

The problem of the flexibility index is formulated as:

F«max6

s.t. maxminmax f,(d,z,0)<O

e«r • jd JV

$$T(\delta) = \{e/e^{N} \text{ -SAT} \le \theta \le \theta^{N} + \delta\Delta\theta^{+}\}, \delta \ge 0 \tag{7}$$

where T(6) is a variable set of parameters, defined through a scalar variable S. This is a quantitative measure of the flexibility of a given design. If F is equal to one, the flexibility objective has ben achieved; if it is larger, the design will be feasible for a wider range of uncertain parameters than the proposed one. If F is less than unity, F gives the measure of the fractional deviation from die nominal condition that can be accommodated by the process.

Solution of (7) is not easy, but it can be decomposed in a two-level optimization problem. For the special case that the functions are mutually 1-D quasi-convex in 6, and quasi-convex in z (for example, linear in z), the critical point 0^c that defines the solution of (7) will be in a vertex of the set T of uncertain parameters T.

For the flexibility index, if critical points can be assumed lying on the vertices of T, then (7) can be simplified as:

F»min5^k

*«v (8)

where 5* is the maximum allowed deviation in each direction A6, k 6 V={k/1 $\le$ k $\le$ 2^m}, given by the non-linear problem:

5^k • max 6

5.2

s.t. fjCd.i.e^SO jeJ (9)

$$\theta^{k} = \theta^{N} + \delta\,\Delta\theta^{k}$$

where z are the control variables and 5* is the displacement in the direction of the vertex k. The control variables z in our problem are the reflux and a product flow rates.

(8) and (9) constitute the basic formulation for the flexibility as shown in Halemane and Grossmaim (1983), and Swaney and Grossmarm (1985)

The inequalities f represent the maximum impurities or minimum purities required in the separation process. The maximum sizes of equipment are also included in these constraints. For example, the area required ($S_{Reqmrcd}$) for cooling should not exceed the condenser area ($S_{Av—abU}$), as shown in the following inequality:

$$(S_{Required}(d, z, \theta^{k}) - S_{Available})_i \le 0 \tag{11}$$

where S indicates size and i is the sub index identifying a given size in the column. If the equipment sizes are known, the bottlenecks are identified with the active constraints related to sizes S_r

The constraints f are nonlinear functions. The NLP sub problem (9) is solved with the successive quadratic programming code OPT of Biegler and Cuthrell (1985).

The product compositions are evaluated using a rigorous simulation code. For the presented example, the SRK equations were used to predict the vapor-liquid equilibria. The composition derivatives with respect to reflux and bottom product flow rate are calculated analytically using the chain rule with elements of the Jacobian generated in the simulation. More information regarding the generation of the analytical derivatives can be found in Hoch (1993] and Hoch and Hiceche(1991).

With the proposed formulation, the analysis of the NLP solution in different directions of the uncertain space gives valuable information. The equipment size that is limiting an increment in the flexibility index is likely to be the bottleneck in the corresponding direction of the uncertain space. It is important to define equipment bottlenecks and the combination of uncertain parameters that will lead to these bottlenecks.

The equipment sizes are assumed to be known, therefore the design bottlenecks are identified as the active constraints related to sizes in the NLP sub problem (9), and which correspond to the worst set of vertices Fl={k / 8* = F}. It may be the case that there is a second set of vertices whose flexibility is dose to the flexibility index, CH = {k/5^{k} «F}$_{9}$ and they should also be studied.

The oversizing of the equipment that is unlikely to be fully used can be determined evaluating the maximum required size of the equipment for the vertices of FI, because the nonacbve constraints related to equipment capacities measures the oversizing.

NUMERICAL EXAMPLE

A debutanizer column of an ethylene plant is chosen to evaluate the design flexibility.

The feed is saturated liquid at IS bar and the column operates at 4 bar. The component feed flow rates in kgmol/h are: propyiene, 0.199, propane, 0.190, n-butane (Ik) 24.706 and n-pentane (hk) 9.875. The total feed flow rate (f) is 34.97. The design specifications included as nonlinear constraints for this problem are shown in table 1.

Table 1: Design specifications

Maximum molar fraction of butane allowed in the bottom product (^{x}c4j)	0.01786
Maximum amount of pentane in the top product (^{x}c3.p)	0.025
Pentane recovery in the bottom product (b_{C5})	0.97

Table 2: Dimensions of the column

Number of rectification stages (Nr)	9
Number of stripping stages (Ns)	10
Diameter of the column (Dcol)	0.634 m
Condenser area (Aeon)	30.9758 m^2
Reboilertret(Areb)	26.8277 m^2

Table 3: Nominal values for the uncertain parameters and their 10% expected deviations.

	Nominal value	Expected deviations	
Condenser best transfer coefficient (Uc)	0.473	±0.0473	[kW/m^C]
Reboiler beat transfer coefficient (Ur)	0.552	±0.0552	fkW/n*:!
Inlet cooling water temperature (Tw)	20	±0.2	rci
Maximum allowed vapor velocity (Ga)	0.380	±0.0380	rm/ti
Butane feed flow rate (Ik)	24.706	±2.4706	[kmol/hl
Pentane feed flow rate (hk)	9.875	±0.9875	[kmol/hi

ACTIVE CONSTRAINTS AND VERTICES ANALYSIS

There are six uncertain parameters, their nominal values and expected deviations shown in table 3. To evaluate the flexibility index, (9) was solved in the 64 vertices of the uncertain space, the control variables being the reflux flow rate (R) and the bottom flow rate (B). The flexibility index is equal to 1.106. meaning that the column operates in the feasible region up to a maximum displacement of 11.06% from the nominal point.

There are three active constraints, two related to the bottom specifications and one to the maximum equipment sizes. The maximum molar composition of butane and pentane recovery in the bottom product are active constraints in the direction of the four vertices. The remaining active constraint indicates that the cooling area required is equal to the available condenser area.

To increase the flexibility index more coding area would be required. An operational bottleneck will be due to the condenser area.

There are four directions in the set FI which have the flexibility index equal to 1.106, shown in table 4. They correspond to the four vertices, where the butane and pentane feed flow rate and the cooling water inlet temperature are equal to their upper bounds and the condenser heat transfer coefficient is equal to the lower bound. This is the worst combination of uncertain parameters for the condenser area, maximum load and cooling water temperature, and minimum heat transfer coefficient. The four vertices correspond to the possible variations of the other two uncertain parameters, the maximum allowed vapor velocity and reboiler heat transfer coefficient, which have no influence on the condenser area.

Table 4: Vertices within the FI set and sizes.

Ur	G*	R	B	6	Aoon	Arab	Dcol
Upper bowl	Upper hound	29.762	10.S31	1.106	X97SS	9.796	0.42SS
Upper bond	Lower boiBd	29.762	10.S31	1.106	J8J7SS	9.796	0.4792
Lewer bound	Upper bouDd	29.762	10.S31	1.106	31J7SS	1X231	0.42SS
Lower bowd	Lower bound	29.762	10.831	1.106	3*975*	12.231	0.4792

For this column, the size that limits an expansion of the feasible region in the uncertain space has been identified. It is also known for which combination of uncertainties it will occur.

Although this combination would be regarded as the worst combination, the values of 5* in the remaining directions give valuable insight of the uncertainty range on the parameters that the column can dealt with being in the feasible space. Such is the case for the set of closest flexibility vertices (CFI), in which the value of 5* is equal to 1.23. It corresponds to four vertices that differ from the vertices in the set FI only because pentane flow rate is on its lower bound rather than in the upper bound. The three active constraints are the same than in the FI vertices.

In the FI directions, feasible operation can be guaranteed up to a distance of 11.06% from the nominal point, while in the CFI directions up to a distance of 12.3%. In both directions, FI and CFI, the values of 5* are similar.

When the butane flow rate is on its lower bound and die pentane feed flow rate is on its upper bound, 5* increases to 1.8. The condenser area is the bottleneck, but obviously with the light key component flow rate decreasing, the cooling load also decreases and *fr* is larger. Then the maximum deviation from the nominal point that allows feasible operation would be 18%. The other two active constraints are the butane impurity in the bottom product and die pentane impurity in the top product, which should also be monitored during the operation. When both feed flow rates decrease, 6* increases up to 2.3. Therefore, in these directions, the column can handle changes of 23% in the uncertain parameters.

The vertex analysis allows the determination of the bottlenecks and quantifies the range of uncertainties that a process can handle in different directions of the uncertain space. This is valuable information regarding the operation of the column.

Knowing that the condenser area is the bottleneck of the column, the flexibility index variations with increments in this area are studied and shown in fig. 1, where is also plotted the variation of the investment cost. The flexibility index is very sensitive to changes in the condenser area for this example. A 10% increment in the condenser area will give a 25% increment in the flexibility index, with a corresponding increment in the investment cost of 1.6%. Redesign actions can be taken from this information.

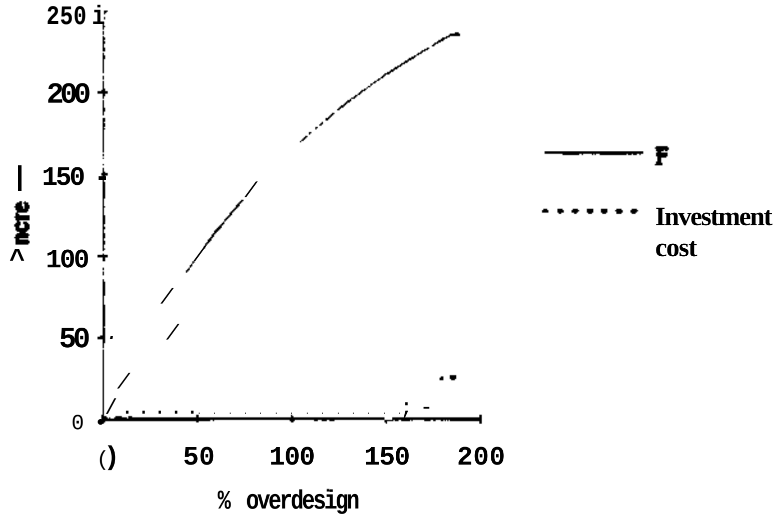

Figure 1: % increment of the flexibility index and investment cost vs. % overdesign of condenser area

CONCLUSIONS

The flexibility analysis coupled with a rigorous simulation of the distillation column quantifies the range of uncertainty that a real process can handle, giving valuable insight on the equipment bottlenecks and the combination of the parameters in which they will occur.

The flexibility index and cost variations with respect to equipment capacities provides valuable information, at the design stage and during operation, regarding the convenience of redesign or retrofitting.

REFERENCES

Biegler L.T. and Cuthrell J. (1985). Improved Unfeasible Path Optimization for Sequential-Modular Simulators II: The Optimization Algorithm. *Comp. and Chem. Eng.* 9, 3.

Fisher W. Doherty M. and Douglas J. (1985). Effect of Overdesign on the Operabihty of Distillation Columns, *I&ECProc. Des. Dev.* 24, pp 593-598.

Grossmann I.E. and Straub D.A, (1991). Recent Developments in the Evaluation and Optimization of Flexible Processes, *Computer Oriented Process Engineering*, Vol 10, pp. 49-59.

Halemane K. and Grossmann I.E.(1983). Optimal Process Design under Uncertainty, *AIChEJ.* 29, 3.

Hoch P. (1993). Diseño Optimo y Flexibilidad de Cohimnas de Destilacidn, PhD Thesis, Universidad National del Sur, Bahia Blanca, Argentina.

Hoch P. and Eliceche AM. (1991). Optimal Design of Non-Conventional Distillation Columns, *Computer Oriented Process Engineering*, Vol 10, pp 369-374.

Hoch P. and Eliceche AM (1994). Sensitivity of Distillation Column Design to Uncertain Parameters, *IChemE Symp Ser.* 133, pp. 459-466.

Kubic W.L. and Stein F.P. (1988) A Theory of Design Reliability using Probability and Fuzzy Sets, *AJChE J.* 34, 4, pp. 583-601.

Swaney R. and Grossmann I.E. (1985). An Index for Operational Flexibility in Chemical Process Design. Pan 1: Formulation and Theory. *AIChE J.* 31, pp. 621-630.