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A Simplified Cost Function for Distillation Systems Evaluation

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The chemical engineer needs a quick and rough economical evaluation to decide between alternative designs and optimize the operating parameters from early stages of design. The ability to find a reasonable optimum operating conditions of a complex distillation system within a short period is difficult due to a huge mathematical computing effort required and mathematical convergence difficulties. This contribution proposes a simplified cost function taking into account the main parameters to which are proportional the capital and operational costs. The goal is not to provide an exact cost estimate in some currency units, the aim of the paper is to provide an optimal operational window defined by a percentage over the minimum cost value. The optimized illustrative example is a pressure-swing distillation system with a reactive column for the transesterification of residual methyl acetate with ethanol to produce ethyl acetate and methanol.

1. Introduction

The first requirement to optimize a process is to define the objective function to minimize, usually a cost function. Cost estimation is a specialized profession. Preparing an estimated cost with an accuracy of ± 5 % is about 2 per cent of the total project cost (Sinnott et al, 1999). The chemical engineer, however, needs a quick and rough economical evaluation to decide between alternative designs and optimize the operating parameters from early stages of design. The preliminary estimates have accuracy typically ±30 % and this accuracy increases to ±10-15 % at the authorization estimates (budgeting).

The total cost is the sum of investment and operational costs. The investment costs must be defined by unit of time before being added to the operational costs. Therefore, the investment costs vary depending on marginal conditions, e.g. the period of depreciation or the consideration of calculated interest, which influences the exact optimum parameters conditions.

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As a reasonable simplification, similar weighting between operating and annualized investment costs can be chosen (Bauer and Stichlmair, 1998). However, after the optimization, Frey et al (1997) obtained that the investment costs were about twice the operational costs. Several optimizations of the same system can provide different optimal conditions. These apparent contradictory results are consequence of the difficult cost evaluation. Several simplifications are assumed, local minimum can be present and it is difficult to assure that the overall minimum is obtained. Preliminary estimations have low accuracy and the overall cost usually is a function with a quite flat minimum that with small variations can provide quite different optimum conditions. Cardoso et al (2000) used simulated annealing and the results present costs of 15.04 and $15.05 \cdot 10^6$ USD/y for a distillation column with 7 and 8 trays, respectively at 1 and 15 atmospheres. The authors concluded also that several feasible designs could be found from 5 to 17 trays with objective functions within 1% of the lowest cost.

Therefore, an estimation of an accurate cost is a tough task but, fortunately, most of the chemical engineering systems present flat minimum cost regions. An optimum operating window for the main variables of a distillation process is useful to provide reasonable values in the early stages of design and a better understanding of the process in the last stages of accurate cost estimation and optimization.

2. Methodology

A compilation of cost data from various sources shows that the next expression can be used for preliminary investment cost estimates (Sinnott et al, 1999):

$$C_e = C \cdot S^n \tag{1}$$

where C_e represents the purchased equipment cost, S represents the characteristic size parameter, C is a cost constant and n is the index for the type of equipment.

A mathematical deduction leads to the main process parameters influencing the characteristic size parameter and operating costs of distillation systems (Bonet et al., 2006). The operational costs (C_o) are proportional to the vapor flow rate inside the column. Applying mass balance in the condenser, the vapor flow rate is related to the distillate flow rate (D) and the reflux ratio (r). The investment costs (C_e) are proportional to the steel required in the column shell and to the thickness of the walls. This leads to the proportionality with the pressure (P), the height of the column, the number of stages (N), the column diameter and the vapour flow rate. The cost expressions are expressed with the proportionality constants (C_1 and C_2) as:

$$C_o = C_1 \cdot \frac{D}{F_c} \cdot (r+1) \tag{2}$$

$$C_e = C_2 \cdot \frac{P}{P_{atm}} \cdot N \cdot \frac{D}{F_c} \cdot (r+1) \tag{3}$$

Equation 2 is adapted to the shape of equation 1 to provide an equipment cost equation taking into account the size of the distillation column.

$$C_e = C \cdot \left(\frac{P}{P_{atm}} \cdot N \cdot \frac{D}{F_c} \cdot (r+1) \right)^n \tag{4}$$

The overall cost is the sum of operational costs and investment costs corrected by some marginal factors, such as the depreciation period, which are included in a constant:

$$C_{OV} = \frac{C}{C_{deprctn}} \cdot \left(\frac{P}{P_{atm}} \cdot N \cdot \frac{D}{F_c} \cdot (r+1) \right)^n + C_1 \cdot \frac{D}{F_c} \cdot (r+1) \tag{5}$$

The exact cost depends on the exact value of the constants that depend on the fluctuations of the steel costs (C), energetic costs (C_1) and of company politics ($C_{deprctn}$). For sake of simplicity, a cost proportional to the total cost is proposed:

$$\frac{C_{OV}}{C_1} = \frac{C}{C_1 \cdot C_{deprctn}} \cdot \left(\frac{P}{P_{atm}} \cdot N \cdot \frac{D}{F_c} \cdot (r+1) \right)^n + \frac{D}{F_c} \cdot (r+1) \tag{6}$$

$$C_{OV} \propto K \cdot \left(\frac{P}{P_{atm}} \cdot N \cdot \frac{D}{F_c} \cdot (r+1) \right)^n + \frac{D}{F_c} \cdot (r+1) \tag{7}$$

The process parameters appearing in the expression (7) can be calculated from shortcut methods such as the infinite/infinite analysis (Bonet et al, 2007; Pleşu et al 2008) and a stage by stage calculation from the feed plate to the distillate and to the bottoms. The values for K and n are estimated from ideal binary mixtures in the present manuscript. The obtained cost function is used in the illustrative example providing the percentage of cost above the minimum cost calculated.

3. Results

The constants K and n depend on equipment type and therefore a distillation column separating ideal binary mixtures is used to determine them. The purity of heavy component in the bottoms is fixed at 0.99 and the purity of the light component in the distillate is fixed at 0.99. The feed composition and the volatility coefficient are the two variables remaining that will be studied and used for the determination of the cost expression parameters. Figure 1 shows that using a reflux 1.3 times the minimum reflux and the fixing the cost expression parameters at K=1.8 and n=0.54, the equipment and operational costs are quite similar for any value of feed composition and for any volatility coefficient. However, Figure 2 shows that the minimum costs are lower than the costs where the operational and equipment costs are equal. The reason is that the equipment cost is a function that decreases more abruptly and with higher slope than the smooth increase of the operational costs. It is noticeable that the optimum cost is very sensitive to small changes of the relative volatility. This behavior is consequence of the flat minimum cost region and of the number of stages that is a discrete variable. Therefore, the value of 0.54 for the constant n is acceptable but the constant K should be twice higher, in this way the results are in accordance with Frey et al. (1997) and the rule of thumb that the optimal reflux is around 1.3 times the minimum reflux (Figure 3).

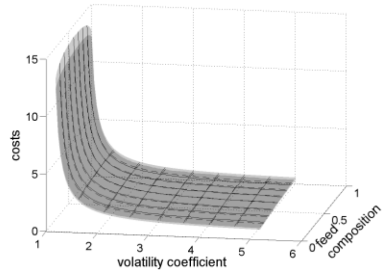

Figure 1: Operational and investment costs for ideal mixtures assuming K=1.8 and n=0.54.

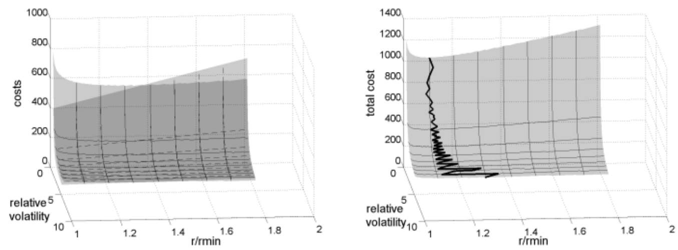

Figure 2: Operational and investment costs crossing point for ideal mixtures assuming K=1.8 and n=0.54.

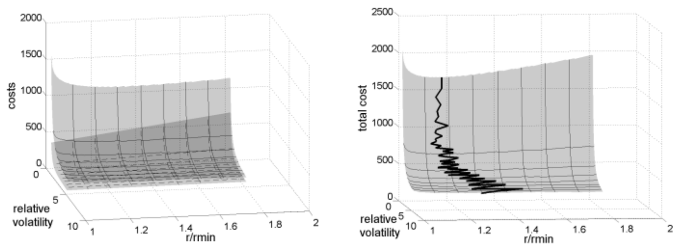

Figure 3: Operational and investment costs crossing point for ideal mixtures assuming K=3.6 and n=0.54.

According to the results, the following cost function is adjusted:

$$C_{OV} \propto 3.6 \cdot \left(\frac{P}{P_{atm}} \cdot N \cdot \frac{D}{F_c} \cdot (r+1) \right)^{0.54} + \frac{D}{F_c} \cdot (r+1) \qquad (8)$$

4. Illustrative example

The illustrative example optimized is a pressure swing distillation system with a reactive column for the transesterification of residual methyl acetate with ethanol to produce ethyl acetate and methanol. Bonet et al. (2007) provide the detailed description of the system discussing its degrees of freedom and the infinite/infinite analysis with the minimum distillate flow rate of the second column (D2min). The second column

distillate (D2), second column distillate composition (xD2) and first column pressure (P) vary without influencing the product purities. These influence mainly the number of stages and reflux required in each column to reach the desired purities. The influence of these three variables on the system performance is studied in the present paper. Notice that any of these three variables affect both columns of the distillation system and therefore the entire system must be optimized at once. The overall cost depends on the sum of both columns; therefore, it is not possible to optimize these parameters taking into account the columns one by one.
The calculations are performed using Simulis Thermodynamics thermophysical properties calculation server available as a MATLAB toolbox. The default thermodynamic parameters of Simulis are used in the calculations, the UNIFAC thermodynamic model being selected.
Figure 4 shows the overall costs versus the operating pressure of the first column. The optimum pressure is around $7 \cdot 10^5$ Pa. The cost 5 % higher than the minimum one can be reached by a pressure value in the range from 4.5 to $12 \cdot 10^5$ Pa. The cost increases exponentially when the pressure of the first column becomes close to the second column pressure. A similar behavior is observed in Figure 5 for D2 and xD2, when they become closer to a minimum value the cost increases abruptly. However, for values higher than the optimum the increase is smooth. The optimum D2/D2min is between 1.55 and 2.35 and the optimum xD2 is between 0.34 and 0.40. Several local minimum are detected. Figure 6 shows the optimal operating window for the variables xD2 and D2/D2min at constant pressure of $7 \cdot 10^5$ Pa. It can be observed that the optimum is just at the limit of an unfeasible zone, therefore the control of the process will have an important role in the choice of these variables.

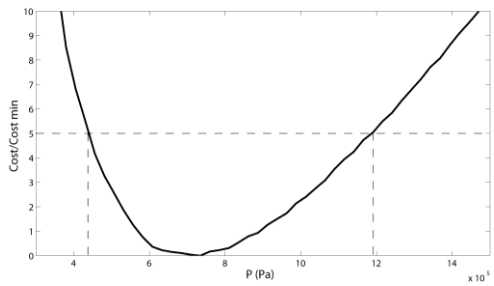

Figure 4: Pressure optimization.

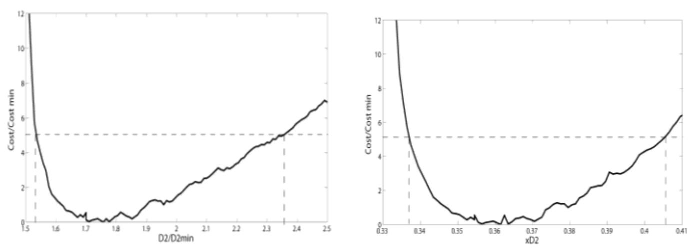

Figure 5: Optimal values of D2 and xD2 at 709 kPa.

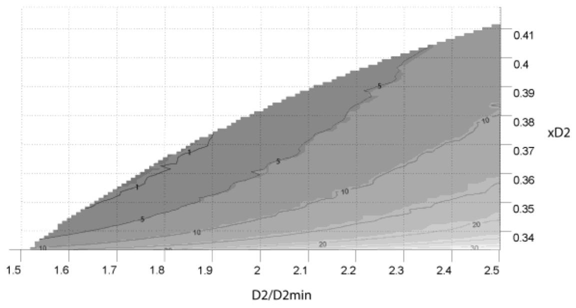

Figure 6: Feasible region and cost contour lines at 709 kPa.

5. Conclusions

A simplified cost function has been proposed and used to evaluate an illustrative example of a complex distillation system. The optimum values for the studied variables are in a quite large optimal operating window. In this particular case, it is noticeable that the optimal operating window is limited by an unfeasible region. The procedure provides values for the main variables of the system at the early stages of design and a guide for further more detailed calculation such as initialization points and a forecast of possible drawbacks.

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