JOINT OPTIMIZATION OF THE CONSTRUCTION AND OPERATION AT VARIOUS PRESSURES OF PLATE DISTILATION COLUMNS

PART I. THE COST FUNCTION

By

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Economical aspects are very important in the design of distillation columns. Economical optimum can be interpreted in several ways, corresponding to the maximization or minimization of various parameters. The diverse definitions of economical optimum lead to different target functions with different variables [1—10].

The most general objective can be defined as the minimum of total or over-all production costs, including investment and operation costs, as a function of design, structural and operational parameters, and the quality and quantity of products. This is overall optimization.

This paper is concerned with the optimization of grid-plate distillation columns, as an example. The cost model, covering all pertinent parameters will be constructed and discussed for this particular case, but the method can be applied to any othei type of plate.

1. *The optimum reflux ratio*

The classical method for the determination of optimum investment and operational parameters of distillation columns consists in calculating the optimum reflux ratio.

This method is based on the following simplifying assumptions:

(1) The theorem of molar evaporation and overflow is valid.

(2) The thermal losses of the column and the pressure drop at the plates are negligible.

(3) The column diameter is calculated from the pre-estimated maximum permissible vapour flow rate at the top of the column, which depends on the construction of plates.

(4) The expectable average efficiency of the column can also be pre-estimated.

(5) The variation in the heat transfer coefficients of exchangers is negligible.

In this work the cost function is based on these classical considerations, but in a more complete and generalized form, omitting the majority of the above assumptions.

It is to be stressed first that the efficiency is considered as a variable, depending on constructional and operational parameters. This way of treatment has so far been ignored in related works, and even when some authors pre-estimated the efficiency, its variation was not taken into account.

As a second difference with respect to previous studies, the design parameters are also regarded as variables in the cost model. Owing to the simplicity of grid plates, the parameters of the plate and the plate spacing can also be directly involved as variables. This treatment allows the joint determination of the optimum reflux ratio and design parameters in optimizing the total costs.

The effect of pressure drop on the plates is also taken into account. This is important when the cost model is applied to vacuum columns used in difficult separation problems.

2. *The distillation problem*

Let us consider a grid-plate distillation column of continuous operation which separates a binary mixture, to produce a distillate of desired composition and quantity. The composition of the feed and the bottom product are given, and the feed plate is optimal. The distillation is performed at the appropriate pressure, and the pressure drop on the plates is also taken into account, if necessary.

These constraints satisfy the definition of the degree of freedom for a two-product distillation column with one feed point, separating a binary mixture [11].

The other data used in the calculations, such as the parameters of the heating steam, cooling water, the over-all heat transfer coefficients of heat exchangers, the temperature of the mixture fed into the pre-heater, etc., are chosen arbitrarily by the designer.

3. *The cost function*

3.1. *Investment costs*

The annual total cost of a distillation column is the sum of the annual fractions of investment and operational costs.

The costs of investment include the costs per annum of the column and its auxiliary equipment, taking into account an annual amortization rate of 10%. As utilities are meant the re-boiler, the total condenser, the pre-heater and the reflux pump which recycles the reflux from the bottom of the column. For non-atmospheric operation the compessor or vacuum pump is also included.

Other extra equipment involved in the analysis would impair generalization. The cost function will be presented for the case of atmospheric operation.

3.1.1. *The investment costs of the column*

The investment costs of a distillation column comprise the cost of the plates and the column shell. Since the phase flow percentages are different between the lower and upper parts of the column, a fact greatly affecting the flow rate and the efficiency, it appeared advisable to evaluate the parameters (vapour density, the value of L/G, vapour flow rate, efficiency, column diameter, etc.) separately for the sections above and below the feed, in order to improve accuracy.

The upper and lower column sections are often hardly different in diameter, and thus it is not absolutely necessary to apply different diameters; a uniform diameter, for instance the larger one, may be chosen. This choice of diameter may, however, cause an underload in the modified section of the column, involving a substantial decrease in efficiency. This problem must be tackled individually for each particular case.

The theoretical plate number can be calculated by various exact and empirical methods. An earlier paper [12] discussed this problem from computerization aspects. It has been shown that with the use of a computer it is most convenient to apply the equilibrium curve in a form where the various sections are replaced by straight lines, and to calculate the plate number by a step by step procedure.

The boiling point curve has been replaced similarly by linear sections in the calculation of average temperatures.

3.1.1.1. *The cost of plates.* The simple geometry of grid plates permits to determine directly the required mass of structural material [1, 2].

The required mass of material, in kilograms, for one plate in the column section above the feed is

$$G_{1t_f} = \frac{d_f^2 \pi}{4} e (1 - F) \varrho \tag{1}$$

Introducing the unit cost E_t (Ft/kg), which is the commercial price of 1 kg of material processed into plate, we obtain the total cost of the plates in the uppor column section:

$$A'_{t_f} = E_t \frac{N}{\eta_f} \frac{d_f^2 \pi}{4} e (1 - F) \varrho \tag{2}$$

The column cross-section area can be calculated from the vapour flow rate and the linear vapour velocity:

$$\frac{d_f^2 \pi}{4} = \frac{V}{v} \tag{3}$$

The "optimum vapour velocity" [13] where column efficiency is maximal [14], and, — as shown in our paper [15], — the material cost is minimal, can be given as

$$v = 6.9\, F \left(\frac{L}{G}\right)^{-0.3} \sqrt{\frac{1.2}{\gamma}} \tag{4}$$

The maximum efficiency [14] is:

$$\eta = 0{,}53 \left(\frac{v^2}{H.g}\right)^{-0.3} \left(\frac{L}{G}\right)^{5.19} \left(\frac{p}{p_0}\right)^{-0.21} \tag{5}$$

To use the above correlations, one must know the mean specific weight of the vapour flow, the average flow rate, and the average of the ratio L/G for the upper column section. The average concentration required to calculate these parameters can be determined from the operating line, by taking an arithmetic mean:

$$y_f = \frac{1}{2} \left(x_D + \frac{R}{R+1} x_F + \frac{x_D}{R+1}\right) \tag{6}$$

Using the ideal gas law, we obtain the average specific weight:

$$\gamma_f = \frac{y_f M_1 + (1 - y_f) M_2}{22.41} \; \frac{273.16}{t_f + 273.16} \; \frac{p}{p_0} \tag{7}$$

where t_f is the boiling point corresponding to the concentration y_f.

The L/G ratio can be expressed as the arithmetic mean of the L/G values at the head and the feed point:

$$\left(\frac{L}{G}\right)_f = \frac{1}{2} \left(\frac{R}{R+1} + \frac{R}{R+1} \; \frac{x_F M_1 + (1 - x_F) M_2}{y_k M_1 + (1 - y_k) M_2}\right) \tag{8}$$

Substituting Eqs. (3 through 8) into Eq. (2) and reducing the constants, we obtain the cost of the plates in the upper column section:

$$A_{t_f} = \mathrm{cg}(R)\, e F^{-0.4} (1 - F)\, H^{-0.3} (R + 1) \frac{1.6}{10} \tag{9}$$

The functional relationship $g(R)$ refers to the reflux dependence of N and t_f, evaluated from the equilibrium and vapour curves approximated with linear sections. The last term 1.6/10 expresses that 60% of the investment costs (and thus, of the corresponging partial costs) are allowed to mounting, instrumentation, etc., and the amortization period is 10 years. This factor also appears in the other investment costs.

The investment cost of the lower column section can be determined by similar considerations.

The sum of these costs is the annual investment cost of the plates:

$$A_t = c_1 r_1(R)\, e\ F^{-0.4}(1 - F)\, H^{-0.3}(R + 1) \tag{10}$$

3.1.1.2. *The costs of the column shell.* The material requirement of an annular portion of the shell in the upper column section, assuming an excess of 10% for the rim, is

$$G_{1k_i} = 1.1\ d_f \pi z H \varrho \tag{11}$$

Introducing the unit cost E_k(Ft/kg), considering the percentage instrumentation and amortization, and substituting Eqs. (3 through 8) into Eq. (11), one obtains the cost of the shell of the upper column section. The lower section can be treated in a similar manner, to obtain the total cost of the column shell:

$$A_k = c_2 r_2(R)\ F^{0.1} H^{0.7}\, z(R + 1)^{0.5} \tag{12}$$

The total cost of the column is the sum of the costs of the plates and the shell jacket.

3.1.2. *Investment costs of auxiliary equipment*

The re boiler, condenser and pre-heater are shell-and-tube heat exchangers. Correlating the data found in the institute standard of the Hungarian Chemical Industries Engineering Centre [16] for heat-exchangers with a length of 3000 mm, we obtained a correlation between the material requirement and the surface of the exchanger:

$$G_h = 80\ F_h^{0.75} \tag{13}$$

The surface area can be calculated from the heat balance of the boiler. The annual investment cost of the boiler, as calculated from the surface area, the unit cost and Eq. (13), can be given as

$$A_{fo} = E_h\, 80 \left(\frac{1000\, D}{k_1(t_g - t_W)}\right)^{0.75} (R + 1)^{0.75}\, \frac{1.6}{10} \tag{14}$$

The surface area of the condenser can be determined from its heat balance.

Substituting this value into Eq. (13), we obtain the annual investment costs of the condenser:

$$A_{ko} = E_h 80 \left(\frac{1000\, D\, \lambda\, ln \frac{t_D - t_1}{t_D - t_1}}{k_2(t_2 - t_2)} \right)^{0.75} (R + 1)^{0.75} \frac{1.6}{10} \tag{15}$$

Reducing the constants to a common factor c_3, the annual investment costs of the boiler and condenser can be expressed as

$$A_{fo} + A_{ko} = c_3(R + 1)^{0.75}$$

The feed is pre-heated to its boiling point by the pre-heater. Its surface area can be determined from the heat balance, and its annual investment cost from Eq. (13). This value is independent of the reflux ratio, and is thus denoted by a constant:

$$A_{el} = c_4 \tag{16}$$

The correlation between the lift and the material requirement of the reflux pump was calculated by correlating the data found in a pump catalogue [17] for a multistage centrifugal pump of type TTM 50:

$$G_{sz} = 40\, H_t^{0.41} \tag{17}$$

The needed reflux pump lift is given by:

$$H_t = \left(\frac{N}{\eta_f} + \frac{M}{\eta_a} \right) (H + e) \tag{18}$$

The annual investment cost of the reflux pump can be determined from Eqs. (5), (17) and (18)

$$A_{sz} = c_5 r_o (R)^{0.41}\, F^{0.246}\, H^{-0.123}\, (H + e)^{0.41} \tag{19}$$

3.2. *Operational costs*

The costs of operation comprise the annual cost of heating steam used in the re-boiler and pre-heater, the cost of the cooling water used in the condenser, and that of the electrical power for operating the reflux pump. For the sake of simplicity it is assumed that saturated steam is applied, by utilizing its heat of condensation.

To calculate the operational cost of the boiler, the required amount of steam was calculated from the heat balance, allowing for a heat loss of 10%.

Assuming 8000 hours of operation per year, the annual cost of steam used in the boiler can be given as

$$A_{g_{f_0}} = E_g\, 8000 \frac{1 \cdot 1\, \lambda\, D}{\lambda_g} (R + 1) \qquad (20)$$

The cooling water consumption in the condenser can be calculated from the balance of the heat of condensation and the heat dissipated by the cooling water. From the balance, the annual cost of cooling water is

$$A_v = E_v \frac{D\lambda}{1000(t_2 - t_1)} (R + 1)\, 8000 \qquad (21)$$

The total annual operation costs of the boiler and condenser can be expressed, reducing the constants in Eqs. (20) and (21) to one constant, c_6, as:

$$A_{g_{f_0}} + A_v = c_6(R + 1) \qquad (22)$$

The annual operation cost of the pre-heater is independent of the reflux, and can therefore be denoted by a constant:

$$A_{g_{el}} = c_7 \qquad (23)$$

The comments regarding the boiler also apply here.

The power required by the reflux pump is a function of the delivered amount, the lift and the efficiency, (again an arbitrary design value):

$$T = \frac{R\, D[x_D M_1 + (1 - x_D)\, M_2]\, H_t\, 9.81}{3600\; 10^6\, \eta_{sz}} \qquad (24)$$

From Eqs (18) and (24), the annual cost of pumping energy is

$$A_e = c_8 r_3(R)\, R\, F^{0.6}\, H^{-0.3}\, (H + e) \qquad (25)$$

The total cost of operation is the sum of the costs of steam, water and electric power.

3.3. *The total cost function*

The sum of the annual percentages of investment and operational costs is the total cost function:

$$K = A + A_k + A_{fo} + A_{ko} + A_{el} + A_{sz} + A_{g_{fo}} + A_v + A_{g_{el}} + A_e \qquad (26)$$

For a grid-plate column this function can be expressed in terms of the constructional parameters (F, H, e, z) and the reflux (R):

$$K = c_1 r_1 e F^{-0.4}(1-F) H^{-0.3}(R+1) + c_2 r_2 F^{0.1} H^{0.7} z \cdot (R+1)^{0.5} + \\ + c_3(R+1)^{0.75} + c_4 + c_5 r_3^{0.41} F^{0.246} \cdot H^{-0.123}(H+e)^{0.41} + c_6(R+1) + \\ + c_7 + c_8 r_3 \cdot R F^{0.6} H^{-0.3}(H+e) r_3 \qquad (27)$$

The problem is now to find the minimum of the total cost function given by Eq. (27) for a particular distillation problem.

Since the original function contains the combinations of various fractional powers of the variables, and so do its derivatives and besides, the variables r are rather complicated functions of the reflux ratio, the system of derivative equations cannot be solved in a closed form.

Investigating the role of each variable, it is readily seen from the form of the function that K increases monotonically with the values of z and e. The costs have, therefore, no extremum with respect to these variables, which assume their structurally lowest permissible value at the optimum. It is sufficient therefore to investigate K as a function of three variables.

The derivatives with respect to F or H contain only negative powers of these variables, and thus at $F = 0$ or $H = 0$ the derivatives tend to infinity. This indicates that the solutions are non-zero. The optimum of reflux ratio R is accordingly at a value higher than minimum.

The mathematical difficulties can be overcome by using computer methods to find the optimum.

The optimum values of parameters may be find by optimization routine programs, but this method gives an insufficient image on the run of the function. To investigate the effect of variables in particular, a computer program yielding the cost at several points over a given range of parameters, selecting, simultaneously, the lowest function value and the corresponding parameters.

In our actual calculations the latter, "natural" method has been applied to study the run of the function. The location of optimum has been checked by an optimization routine program, based on the "simplex" principle. The optima determined by the two programs were indentical in every case.

The cost function proved to be suitable for the optimization of the distillation costs of various binary mixtures, different in behaviour over a wide range of relative volatilities. The results will be given in Part II of this serie.

Summary

A model has been constructed for the simultaneous treatment of operational and investment costs of distillation columns. The model comprises the design parameters, and the dependence of separation efficiency on various fectors, and it can be used to determine the joint optimum of these parameters. As a starting point, the vapour velocity belonging to maximum efficiency has been chosen for a grid-plate column.

Notation

A_e annual cost of electric power (Ft/year)
A_k investment cost of the column shell (Ft/year)
A_t investment cost of column plates (Ft/year)
A_v annual cost of cooling water (Ft/year)
A_{el} investment cost of pre-heater (Ft/year)
A_{fo} investment cost of re-boiler (Ft/year)
A_{ko} investment cost of condenser (Ft/year)
A_{sz} investment cost of reflux pump (Ft/year)
A_{gel} annual cost of heating steam for the pre-heater (Ft/year)
A_{gfo} annual cost of heating steam for the boiler (Ft/year)
A_{tf} investment cost of the plates in the upper column section (Ft/year)
A'_{tf} price of plates in the upper column section (Ft)
$c, c_1, c_2, \ldots, c_8$ constants
d_f the inner column diameter in the upper section (m)
D the amount of distillate (kmol/h)
e thickness of a grid plate (m)
E_g unit cost of heating steam (Ft/tons)
E_h unit cost of material processed as heat exchanger (Ft/kg)
E_k unit cost of material processed as column shell (Ft/kg)
E_t unit cost of material processed as plate (Ft/kg)
E_v unit cost of cooling water (Ft/1000 m^3)
F free cross-section of grid plate (m^2/m^2)
F_h surface area of heat exchanger (m^2)
g gravity acceleration (m/s^2)
G_h mass of material for the heat exchanger (kg)
G_{sz} mass of material for the pump (kg)
G_{1kf} mass of material for an annular portion of shell in the upper column section (kg)
G_{1tf} mass of material for one grid plate in the upper column section (kg)
H plate spacing (m)
H_t column height (m)
k_1 heat transfer coefficient of re-boiler (kcal/m^2h °C)
k_2 heat transfer coefficient of condenser (kcal/m^2h °C)
K total cost (Ft/year)
L/G ratio of vapour to liquid flow in the column (kg h^{-1}/kg h^{-1})
$(L/G)_f$ ratio of vapour to liquid flow in the upper column section (kg h^{-1}/kg h^{-1})
M theoretical plate number in the lower column section
M_1 molecular weight of the more volatile component (kg/kmol)
M_2 molecular weight of the less volatile component (kg/kmol)
N theoretical plate number in the upper column section
p column pressure (atm)
p_0 atmospheric pressure (atm)
$r_1(R)$ function of reflux ratio
$r_2(R)$ function of reflux ratio
$r_3(R)$ function of reflux ratio
R reflux ratio
t_1 temperature of cooling water before the condenser (°C)
t_2 temperature of cooling water after the condenser (°C)
t_D boiling point of distillate (°C)
t_f average temperature in the upper column section (°C)
t_g temperature of saturated heating steam (°C)
t_W temperature of the residue (°C)
T power consumption of reflux pump (MW)
v vapour velocity related to the entire cross-section of the column (m/s)
V vapour flow in the column (m^3/s)
x_D concentration of distillate (mol/mol)
x_F concentration of feed (mol/mol)
y_f average vapour concentration in the upper column section (mol/mol)
y_k vapour concentration at the feed (mol/mol)
z wall thickness of the column (m)

Greek symbols

γ specific weight of ascending vapour (kp/m^3)
γ_f average specific weight of ascending vapour in the upper column section (kp/m^3)
η column efficiency
η_a column efficiency in the lower section
η_f column efficiency in the upper section
η_{sz} efficiency of reflux pump
λ average heat of vaporization of the mixture (kcal/mol)
λ_g heat of vaporization of heating steam (kcal/kg)
ϱ density of structural material (kg/m^3)

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