JOINT OPTIMIZATION OF THE CONSTRUCTION AND OPERATION AT VARIOUS PRESSURES OF PLATE DISTILLATION COLUMN

PART II. DISCUSSION AND GENERALIZATION OF RESULTS

By

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Part I of this series had been concerned with the total cost function of grid-plate distillation equipment, taking the construction and operation parameters simultaneously into account. The total cost function, i.e. the sum of annual investment and operation costs, was given as a function of the free cross-section of the plates F, the plate spacing H, the wall thickness of the column z, the plate thickness e and the reflux ratio R:

$$K = f(F, H, z, e, R). \quad (1)$$

The optimum of costs is determined by finding the minimum of K within the given limits of variables.

The calculations were performed on a GIER digital computer. The minimum was searched by a mapping method, with cyclic variation of the parameters within the limits, and the cost function was evaluated at several points. In addition to selecting the minimum value and its parameters, this procedure also provides an image on the run of the function. The location of optimum was checked by an optimization routine program, based on the simplex principle. The locations of optima were invariably identical to those found with the other program.

Using the cost function, the distillation costs of various binary mixtures have been optimized, where the relative volatilities of the mixtures varied over a wide range. For the sake of comparison, the distillation task was assumed to be the same in each case (see Table 1).

The data characterizing the operation of auxiliary equipment were taken from handbooks (M_1, M_2, λ, c_p, etc.), or given on the basis of empirical values (k_1, η_{sz}). The unit prices (E_t, E_k, etc.) were kindly offered by the Hungarian Chemical Industries Engineering Centre (see Table 1).

The constructional factors irrelevant for the separation, such as the thickness of plates and the jacket, were chosen on the basis of structural and production technological considerations, and the correctness of assumptions was checked by calculations [11].

The expected ranges of plate spacing, free plate cross-section, and reflux ratio were assumed on the basis of the operation parameters of the column.

1. *Atmospheric pressure*

Optimum parameters have been determined for the atmospheric separation of the following mixtures:

n-heptane — methylcyclohexane
carbon tetrachloride — benzene
cyclohexane — *n*-heptane
benzene — toluene
ethanol — water

The optima determined by calculations show strict regularities (see Table 2 and Fig. 1).

Table 1

Data for the computer treatment of cost function

		n-Heptane—methyl-cyclohexane $\alpha = 1.083$	Carbon tetrachloride—benzene $\bar{\alpha} = 1.11$	Cyclohexane—*n*-heptane $\bar{\alpha} = 1.82$	Benzene—toluene $\alpha = 2.47$	Ethanol—water —
D	kg/h	5000	5000	5000	5000	5000
x_F	mol/mol	0.5	0.5	0.5	0.5	0.37
x_D	mol/mol	0.99	0.99	0.99	0.99	0.83
x_W	mol/mol	0.01	0.01	0.01	0.01	0.01
M_1	kg/mol	100.2	153.84	84.16	78	46
M_2	kg/mol	89.18	78.11	100.2	92	18
λ	kcal/mol	7.597	7.08	7.422	7.67	9.5
t_0	°C	20	20	20	20	20
c_p	kcal/kg °C	0.51	0.3225	0.55	0.43	0.92
t_g	°C	119.62	119.62	119.62	119.62	119.62
λ_g	kcal/kg	526.4	526.4	526.4	526.4	526.4
t_1	°C	20	20	20	20	20
t_2	°C	40	40	40	40	28
k_1	kcal/m²h °C	1000	1000	1000	1000	1000
k_2	kcal/m²h °C	500	500	500	500	500
z	mm	10 and 15	10 and 15	10 and 15	10 and 15	10 and 15
e	mm	5	5	5	5	5
ϱ	kg/m³	7800	7800	7800	7800	7800
η_{sz}		0.6	0.6	0.6	0.6	0.6

Table 1 (continued)

p	= 20 atm. ethane—ethylene system
D	= 5000 kg/h
x_F	= 0.5 mol/mol (t = −20 °C)
x_D	= 0.99 mol/mol (t = −28.8 °C)
x_W	= 0.01 mol/mol (t = − 6.8 °C)
λ	= 2.233 kcal/mol
$\varkappa$	= 1.225
z	= 20 and 30 mm
e	= 5 mm
ϱ	= 7800 kg/m³
η_{sz}	= 0.6
η_{ko}	= 0.75

The data of the cooling system (entrance and exit temperatures, heat transfer coefficients, etc. of various heat exchangers) were calculated on the basis of [4, 5 and 6].

p_0	= 100 torr water— heavy water system
D	= 4.989 10⁴ kmol/day (Refs. [13 and 14])
x_F	= 0.99985 mol/mol
x_D	= 0.99995 mol/mol } (Refs. [14, 18 and 19])
x_W	= 0.99 mol/mol
λ	= 10.51 kcal/mol
t_0	= 20 °C
t_g	= 120 °C
λ_g	= 526 4 kcal/kg
t_1	= 20 °C
t_2	= 40 °C
k_1	= 2000 kcal/m²h°C
k_2	= 1500 kcal/m²h°C
z	= 20 and 30 mm
e	= 5 mm
ϱ	= 7800 kg/m³
η_{sz}	= 0.6

Unit costs

Plate:	E_t	= 120 Ft/kg
Jacket:	E_k	= 160 Ft/kg
Heat exchanger:	E_h	= 52 Ft/kg
Pump:	E_{sz}	= 400 Ft/kg
Steam:	E_g	= 120 Ft/tons
Cooling water:	E_v	= 650 Ft/10³ m³
Electric power:	E_e	= 650 Ft/MWh
Compressor:	E_{ko}	= 43 Ft/kg
Vacuum pump:	E_{va}	= 18 Ft/kg

a) The optimum values of *reflux ratio* are very close to minimum (Fig. 1). Irrespective of the relative volatility, the ratio is approximately

$$\sigma = R_{\text{opt}}/R_{\text{min}} \approx 1.05$$

This result is less than the well known and applied approximate rule, i.e. $R_{\text{opt}}/R_{\text{min}} = 1.2 \sim 1.5$. The low value of σ can well be interpreted by considering that the production costs of grid plates are low, and thus the invest-

Table 2
Optimum column parameters calculated with the cost function $p = 1$ atm

	R	R/R_{min}	F m^2/m^2	H m	e mm	z mm	Total cost	Investment cost	Operation cost	Number of real plates		
							10^6 Ft/year			total	upper	lower
n-heptane—methylcyclohexane	24.78	1.050	0.3	0.2	5	10	29.54	6.209	23.33	611	340	271
	24.78	1.050	0.3	0.2	5	15	30.93	7.597	23.33	611	340	271
Carbon tetrachloride —	20.13	1.048	0.3	0.2	5	10	14.93	3.327	11.60	482	373	109
benzene	20.13	1.048	0.3	0.2	5	15	15.77	4.170	11.60	482	373	109
Cyclohexane —	2.618	1.054	0.3	0.2	5	10	5.076	0.634	4.442	178	150	28
n-heptane	2.618	1.054	0.3	0.2	5	15	5.233	0.790	4.442	178	150	28
*$\alpha = 1.82$	2.618	1.054	0.3	0.2	5	10	5.123	0.681	4.442	192	161	31
	2.618	1.054	0.3	0.2	5	15	5.297	—	—	192	161	31
Benzene —	1.353	1.042	0.3	0.2	5	10	3.718	0.536	3.182	176	149	27
toluene	1.373	1.054	0.3	0.2	5	15	3.838	0.635	3.203	165	140	25
*$\alpha = 2.47$	1.353	1.042	0.3	0.2	5	10	3.727	0.545	3.182	176	149	27
	1.373	1.054	0.3	0.2	5	15	3.850	0.647	3.203	165	140	25
Ethanol—water	1.297	1.040	0.3	0.2	5	10	8.735	0.708	8.026	215	206	9
	1.297	1.040	0.3	0.2	5	15	8.897	0.870	8.026	215	206	9
$p = 20$ atm												
Ethane—ethylene	4.48	1.054	0.2	0.2	5	15	8.772	1.385	7.387	168	136	32
	4.48	1.054	0.2	0.2	5	10	8.776	1.393	7.382	132	107	25
$p_0 = 100$ torr												
Water — heavy water	16.99	1.015	0.3	0.2	5	20	1028	125	903	1017	295	722
	17.05	1.019	0.3	0.2	5	30	1048	142	906	986	290	696

The equilibrium curve has been approximated with linear sections; for the mixtures denoted by an asterisk, α was omitted.

ment is much lower than the costs of operation (about 10 to 20%), involving a shift of optimum towards smaller reflux ratios.

The results of recent investigations and computer studies also support that the optimum is close to the minimum value. This qualitative result has been found by FAIR and BOLLES [1]: $\sigma = 1.05$ and ALEKSANDROV [24]: $\sigma = 1.09$. Furthermore, PLATONOV and BERGO [2] obtained $\sigma = 1.092$ for the atmospheric distillation of the multicomponent system ethylbenzene-(*o*-, *m*-, *p*-)xylene (see Fig. 1). Similar value ($\sigma = 1.07$) is found by GROYSMAN [25] too for optimizing a butane–isobutane system using heat pump.

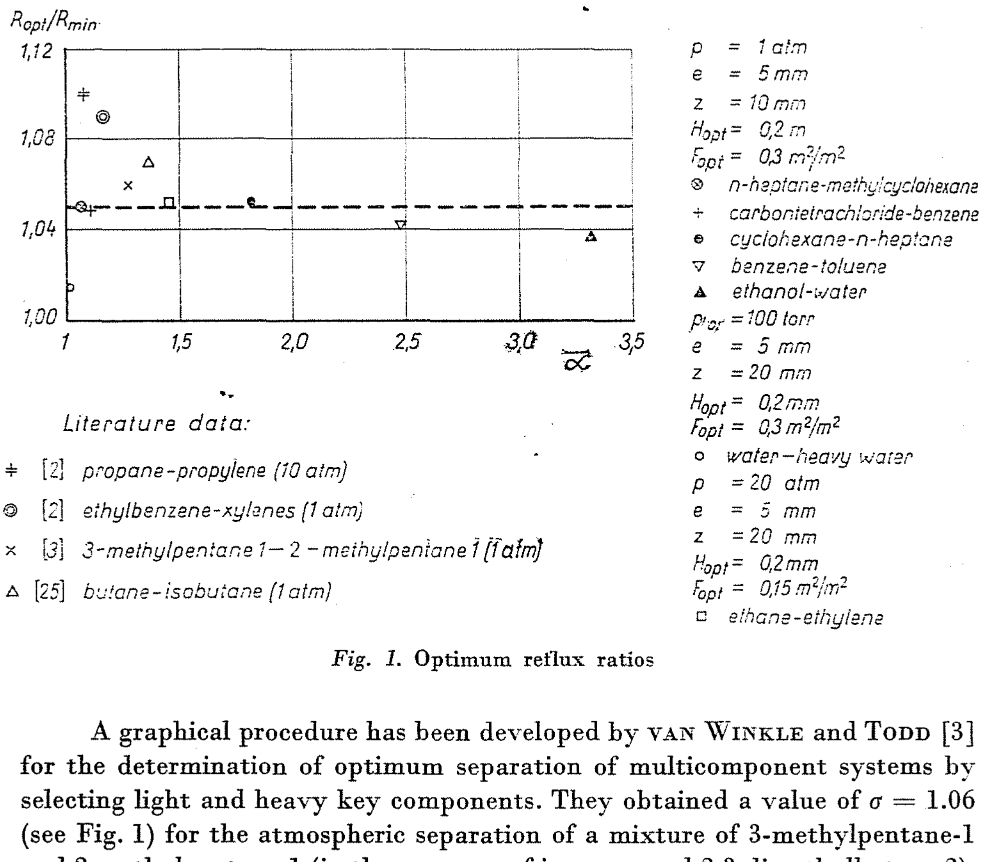

Fig. 1. Optimum reflux ratios

A graphical procedure has been developed by VAN WINKLE and TODD [3] for the determination of optimum separation of multicomponent systems by selecting light and heavy key components. They obtained a value of $\sigma = 1.06$ (see Fig. 1) for the atmospheric separation of a mixture of 3-methylpentane-1 and 2-methylpentane-1 (in the presence of isoprene and 2,3-dimethylbutene-2).

b) The optimum of *plate spacing* always proved to be the smallest permissible, where entrainment and foaming do not affect the separation. At larger spacings the column height increases to an extent not offset by the improvement of efficiency through a decrease in the number of real plates.

c) The optimum of *free cross-section* of plates was always found to be 0.3 m²/m².

Calculations were also performed on the optimization of plate distillers operating at higher than atmospheric pressures and in vacuum. The fundamental problem was, in both cases, the treatment of the pressure-dependent terms of the cost function. The mixture to be separated and the operating pressure were fixed before optimization, which has reduced the generality both in the construction of cost function and in the interpretation of results.

2. *Higher than atmospheric pressures*

The distillation of an ethane–ethylene mixture at 20 atm was studied. On the basis of literature data [4 to 8] two-stage compression was assumed.

The effect of higher pressures appears in the cost function at the following points.

1. The wall thickness of the column must be greater than that of those operating at atmospheric pressure [11], depending on the actual operating pressure.

2. The plate efficiency, and consequently, the column height, is also pressure dependent (see Eq. (5) in Part I, for $p \neq p_0$).

3. An additional cost of the compressors is superimposed on the costs of atmospheric distillation. Correlating the data of the institute standard of Hungarian Chemical Industries Engineering Centre concerning compressors [12], a correlation has been set up between the performance and the material demand of compressors. Accordingly,

$$G_k = 0.58\, T^{0.94} \tag{2}$$

where the performance of the compressor is expressed as

$$T = \frac{\varkappa}{\varkappa - 1} \frac{W_{ko}}{\eta_{ko}} 0.082(273 \cdot 16 + t)\left[\left(\frac{p_2}{p_1}\right)^{\frac{\varkappa-1}{\varkappa}} - 1\right] \tag{3}$$

4. An additional heat exchanger is used to cool the feed after compression, and its cost also appears besides that of the prehe-ater, condenser and re-boiler.

5. The transport height of reflux pump also depends on the pressure through the variable height of the column.

The distillation of ethane-ethylene mixture is performed at very low temperatures, even when the pressure is high, and thus the re-boiler must be operated with refrigerating liquid, and in the "pre-heater" pre-cooling takes place. Consequently, no heating steam is required. The distillate and the feed are chilled with a liquid which can be used at temperatures lower than the freezing point of water. For this purpose a compressed ethane–ethylene mixture or liquid ammonia can be used to advantage [5 to 7]. (The cost of chilling liquid adds to the cost of compressor. According to our calculations the use of ammonia is more profitable.)

The following operation costs are expressly pressure-dependent:

1. The energy consumption of the reflux pump, due to the pressure-dependent variation of plate efficiency, and therefore, of column height.

2. The energy consumption $T_{ko} = 15.2 \; 10^{-6} \; T$ of the compressor, as indicated in [12].

3. To a certain extent, the amount of water required for cooling after compression.

The extremum of the cost function modified with the above factors was determined by a computer.

The results are in a good agreement with those obtained for atmospheric distillation:

a) the optimum *plate spacing* is again at the minimum permitted value, $H_{\text{opt}} = 0.2$ m,

b) the optimum *free cross-section* is, however, $F_{\text{opt}} = 0.15$,

c) the optimum *reflux ratio* is $R_{\text{opt}} = 1.054 \; R_{\text{min}}$.

It is noted that a value of $R_{\text{opt}} = 1.09 \; R_{\text{min}}$ was obtained by Platonov and Bergo [2] for the distillation on a propane–propylene mixture at 10 atm.

3. *Vacuum distillation*

The rectification of a water–heavy- water system at reduced pressure was investigated. The optimization concerned a three-column process, based on the data found in the literature. The top pressure in the column was taken as $p_0 = 100$ torr, assuming a pressure drop of 2 torr pro theoretical plate number [13 to 19]. At such a low pressure the change in relative volatility with the variation of column pressure is not negligible any more.

The cost function pertaining to atmospheric pressure is modified as follows.

1. One must take into account the pressure dependence of the minimum reflux ratio.

When the feed is at boiling point, the minimum reflux ratio is:

$$R_{\text{min}} = \frac{x_D - y_F}{y_F - x_F} \tag{5}$$

To calculate y_F, the α value must be determined at the feed point, where the actual pressure is unknown. The only known fact is that at this point the pressure is higher than the top pressure, namely there is pressure drop. Substituting the known expression

$$y_F = \frac{\alpha x_F}{1 + (\alpha - 1) x_F} \tag{6}$$

into Eq. (5), we obtain

$$R_{\min} = \frac{x_D - x_F}{x_F (1 - x_F)(\alpha - 1)} - \frac{1 - x_D}{1 - x_F} \tag{7}$$

As α decreases with an increase of pressure, it is obvious from Eq. (7) that at increasing pressures $R_{\min}$ also increases. The minimum reflux calculated for the top pressure will therefore be certainly smaller than the "real" minimum reflux, i.e. the reflux for which the calculated theoretical plate number is just infinite, but for an arbitrarily higher reflux it is already finite. On this basis, the "real" minimum reflux is determined by iteration, starting from the value taken at the top pressure. As a real $R_{\min}$ the maximum value of reflux has been chosen for which "infinite" theoretical plate number — in our calculations greater than 500 — is obtained.

2. The modifications in the investment costs arising from the low pressure in the column (wall thickness, plate efficiency, column height, costs of reflux pump) are treated in the same manner as in the calculations of high-pressure distillation [11].

3. A pressure-dependent investment, occurs peculiar for vacuum distillation, is the cost of vacuum pump. Taking into account the data concerning vacuum pumps [21], a correlation was established between the weight and the performance of vacuum pumps:

$$G_{va} = 2.6\, q^{0.54} \tag{8}$$

the performance being:

$$q = \frac{w}{\gamma} \left(\frac{N}{\eta_f} + \frac{M}{\eta_a} \right) \pi \tag{9}$$

The pressure-dependent terms of operation costs (power consumption of the reflux and vacuum pumps) were determined in a manner similar to high-pressure distillation.

The following conclusions could be drawn:

a) the optimum of *wall thickness* is always at the lowest permissible value (20 mm),

b) the optimum *plate spacing* is also at the permissible minimum: $H_{\text{opt}} = 0.2$ m; the result is identical to that obtained for atmospheric and high-pressure distillation;

c) the optimum of *free cross-section* for columns of industrial size is at $F_{opt} = 0.3\ m^2/m^2$, in agreement with the outcome for atmospheric distillation;

d) the optimum *reflux ratio* is $R_{opt}/R_{min\ act.} = 1.015$ for column I in the three-column system [18, 19], which concentrates sea water up to 1%, and is the most expensive column (Fig. 2). For the other columns the optimum of the reflux was so close to the actual minimum that it could not be calculated with a sufficient accuracy.

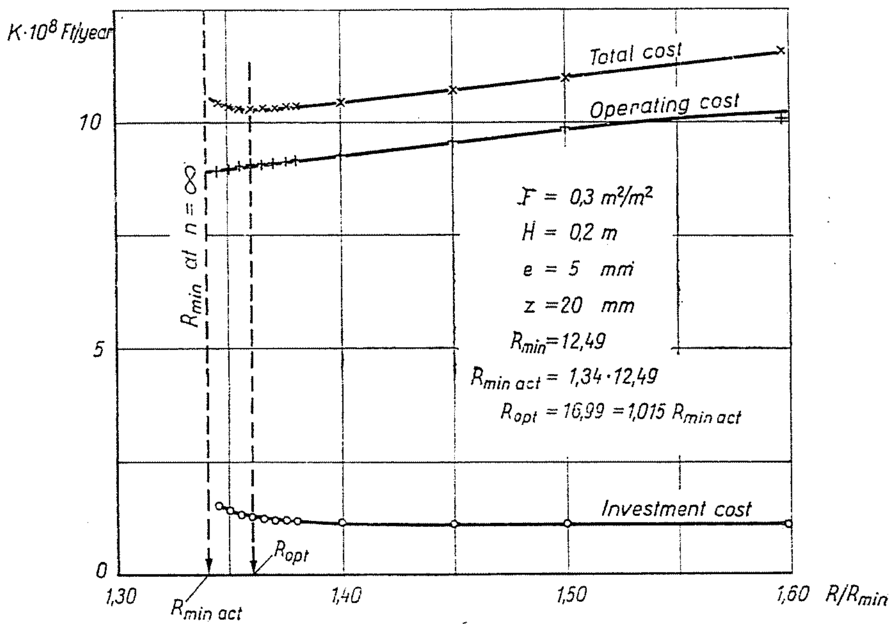

Fig. 2. The separation of water–heavy- water system

4. *A comparison of results to other investigations*

For sake of comparison, calculations were performed by the method of HAPPEL [23], and by the graphical method of VAN WINKLE and TODD [3], using identical initial conditions. The comparison must be restricted to reflux ratios, because the above methods, while taking into account the cost parameters, are inapplicable to determine the joint optimum of constructional and operational parameters.

The $\sigma = R_{opt}/R_{min}$ values obtained by these methods have been compiled in Table 3.

The values calculated by Happel's method [23] are seen to be in good agreement with our result, whereas the method of van WINKLE and TODD [3] gives slightly higher ratios, but the difference is still immaterial.

Table 3

Comparison of $\sigma = R_{opt}/R_{min}$ obtained by various methods

	Cost function this work	Happel, van Winkle, Todd	
		[23]	[3]
Benzene—toluene	1.042	1.037	1.08
Cyclohexane—n-heptane	1.054	1.045	1.09

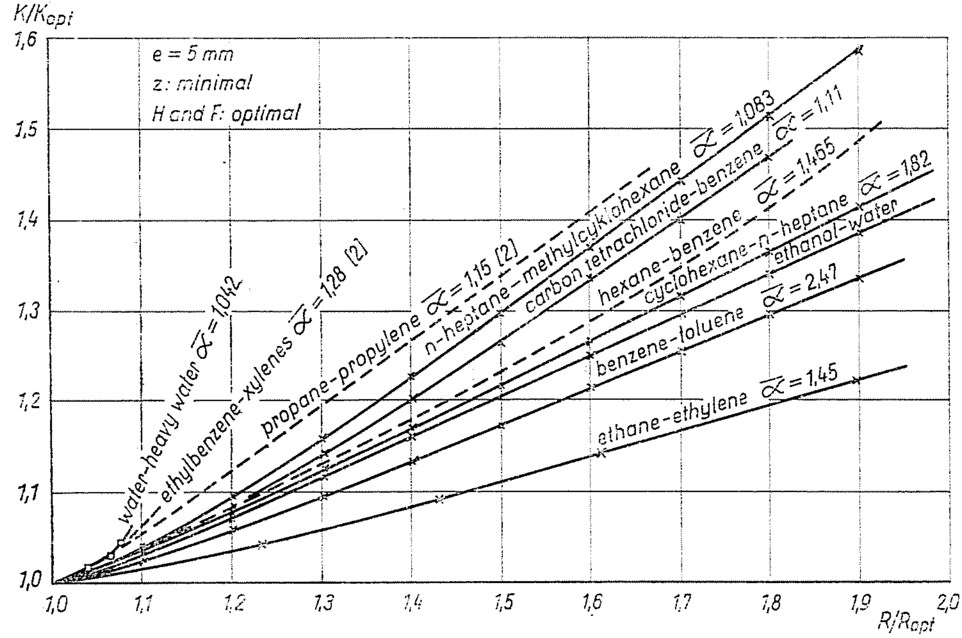

Fig. 3. Relative increase in cost at reflux ratios higher than R_{opt}

5. *Generalization of results*

Having in mind that it may be difficult to maintain the reflux at the optimum ratio since it is very close to the minimum, the application of a higher than optimum reflux ratio may become necessary. The discussed total cost function allows to determine the increase of the minimal total costs at the actual reflux ratio.

The calculations refer to atmospheric operations, and the total cost is treated as a function of reflux ratio at fixed construction parameters (Fig. 3). The ordinata represents K/K_{opt}, i.e. the increase in cost with respect to the minimum total production cost of 1 kilogram of distillate, and the abscissa represents R/R_{opt}, i.e. the excess of reflux with respect to R_{opt}. The mixtures are also characterized by their relative volatilities.

At a particular reflux, Fig. 3 shows the excess of cost to increase substantially with the decrease of relative volatility. No such behaviour is shown by the ethanol–water system, for which it would be a coarse approximation to be characterized by an average relative volatility, and for which the above initial conditions are anyway not valid. The diagrams also show the literature data which were discussed above.

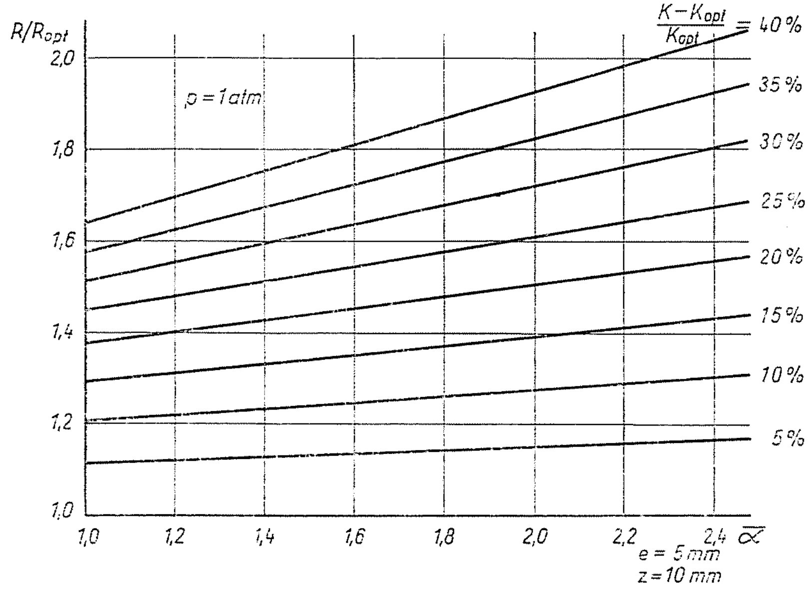

Fig. 4. Percentage increase in cost at reflux ratios higher than R_{opt}.

Using the points belonging to the same R/R_{opt} values, the optimum excess of reflux was plotted vs. $\bar{\alpha}$ for the *n*-heptane–methylcyclohexane, carbon tetrachloride–benzene, cyclohexane–*n*-heptane and benzene–toluene mixtures, which exhibit strict regularities in the increase of costs. The parameter was the percentage increase in cost with respect to the minimum. The points belonging to the same parameters yield a series of straight lines (Fig. 4). In the case of higher relative volatilities a greater practical reflux ratio is seen to be permitted without a substantial increase in costs. Thus, for instance, for a column of optimum construction operated at a reflux of $R = 1.4\ R_{opt} = 1.47\ R_{min}$, the minimum total cost is exceeded by about 18% when the relative volatility of the mixture is $\alpha = 1.5$, but only by about 15% for $\alpha = 2.1$.

Summary

The cost model discussed in Part I of this series has been applied to optimize distillation columns for the separation of various binary mixtures in a wide range of pressures. By generalizing the results, approximate correlations have been set up between the optimum and minimum reflux, and between various parameters and the excess cost of columns operated at reflux ratios higher than minimum.

Notations

c_p	specific heat capacity of feed (kcal/kg °C)
d_a	column diameter in the lower section (m)
d_f	column diameter in the upper section (m)
D	amount of distillate (kmol/h)
e	plate thickness (m)
E_e	unit cost of electric power (Ft/MWh)
E_g	unit cost of heating steam (Ft/tons)
E_h	unit cost of construction material processed into heat exchanger (Ft/kg)
E_k	unit cost of construction material processed into column shell (Ft/kg)
E_t	unit cost of construction material processed into grid plate (Ft/kg)
E_r	unit cost of cooling water (Ft/1000 m³)
E_{sz}	unit cost of construction material processed into pump (Ft/kg)
E_{ko}	unit cost of construction material processed into compressor (Ft/kg)
E_{va}	unit cost of construction material processed into vacuum pump (Ft/kg)
F	free cross-section of grid plate (m²/m²)
F_{opt}	optimal free cross-section of grid plate (m²/m²)
G_{ko}	mass of construction material required for the compressor (kg)
G_{va}	mass of construction material required for the vacuum pump (kg)
H	plate spacing of the column (m)
H_{opt}	optimal plate spacing of the oclumn (m)
k_1	heat transfer coefficient of the reboiler (kcal/m² h °C)
k_2	heat transfer coefficient of the condenser (kcal/m² h °C)
K	total cost (Ft/year)
K_{opt}	optimal (minimum) total cost (Ft/year)
M	theoretical plate number in the column section below the feed
M_1	molecular weight of the more volatile component (kg/mol)
M_2	molecular weight of the less volatile component (kg/kmol)
N	theoretical plate number in the column section above the feed
p_1	pressure before compression (atm)
p_2	pressure after compression (atm)
p_0	top pressure in the column (torr)
q	performance of vacuum pump (litre/min)
R	reflux ratio
R_{min}	minimum reflux ratio
R_{opt}	optimum reflux ratio
t	temperature of the gas to be compressed (°C)
t_0	temperature of the feed (°C)
t_g	temperature of the heating steam (°C)
t_1	temperature of the cooling water fed into the condenser (°C)
t_2	temperature of the cooling water leaving the condenser (°C)
T	performance of the compressor (m³ atm/h)
T_{ko}	power consumption of the compressor (MW)
w	amount of leaking air + entrained vapour (pond/min m of sealing)
W_{ko}	amount of gas to be compressed (kmol/h)
x_D	concentration of the distillate (mol/mol)
x_F	concentration of the feed (mol/mol)
x_W	concentration of the residue (mol/mol)
y_F	concentration of the vapour in equilibrium with the feed (mol/mol
z	wall thickness of the column (m)

Greek symbols

α relative volatility
$\bar{\alpha}$ average relative volatility
γ specific weight of the gas to be pumped (pond/litre)
η_a column efficiency in the lower section
η_f column efficiency in the upper section
η_{ko} efficiency of the compressor
η_{sz} efficiency of the pump
$\varkappa$ c_p/c_v the ratio of heat capacities at constant pressure and constant volume of the gas to be compressed
λ average heat of vaporization of the mixture (kcal/mol)
λ_g heat of vaporization of heating steam (kcal/kg)
ϱ density of the construction material of the column (kg/m^3)
$\sigma = R_{opt}/R_{min}$

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