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CONSTRAINT CONTROL OF DISTILLATION PROCESSES

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Abstract—There is a growing interest to design and operate chemical processes for reduced energy consumption As an example a comparison is made between the distillation of binary mixtures in a conventional distillation column, a vapour recompression system and a two column heat integrated system For all three configurations constraint control schemes are proposed Utility costs can be reduced with about a factor of two by using a heat integrated system

1 INTRODUCTION

In the way it is commonly applied in the chemical industry, distillation is an energy consuming process heat is added in order to evaporate and distill a mixture and cooling has to be introduced to withdraw the added energy (Fig 1) It should come as no surprise that ideas have been proposed to decrease energy consumption in distillation [1–4] One system which was designed to conserve energy was the use of a heat pump by using the heat of condensation of overhead vapour for reboiling (Fig 2) The attractiveness of this option entirely depends on the thermodynamic efficiency of the heat pump

Another way to conserve energy is to replace a single column by two heat integrated columns in parallel, as shown in Fig 3 The overhead vapour from the first column is used as a heating medium for the second column reboiler The first column must be operated at a higher pressure than the second column because the bottom of the second column will be richer in higher boiling components than the top of the first column, and a temperature difference is required for heat transfer

In this paper optimal operation of the different configurations for distillation will be studied starting from a more or less optimal design Optimization of a process generally means operation in the best possible way, consistent with a defined objective and within given constraints [5, 6] This will be demonstrated for the distillation of two binary mixtures propane/propene and butane/isobutane

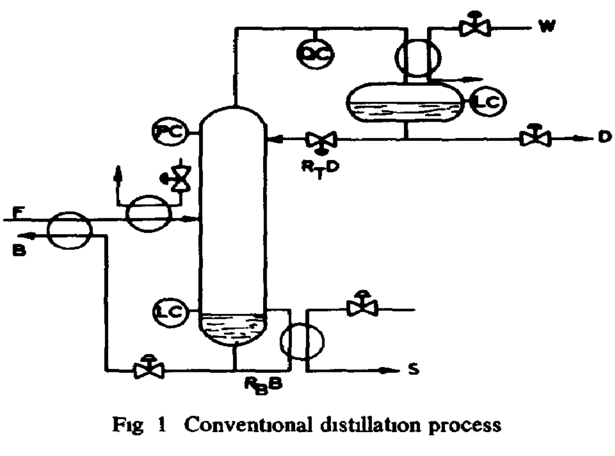

Fig 1 Conventional distillation process

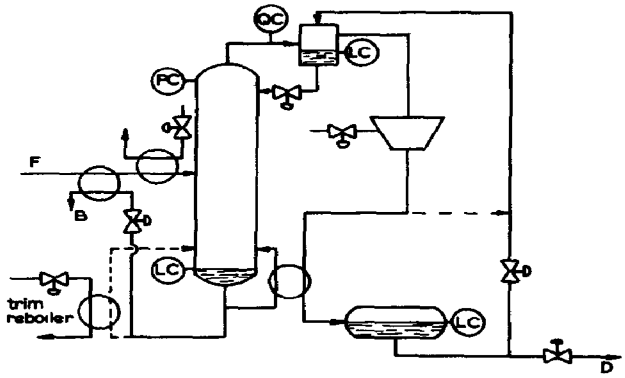

Fig 2 Distillation with vapour recompression

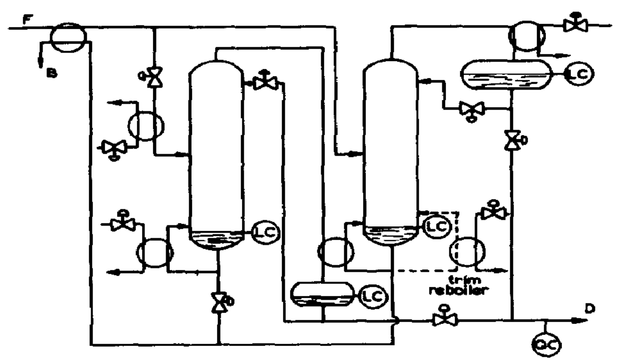

Fig. 3 Distillation with integrated reboiler/condensor

2 DEFINITION OF THE OBJECTIVE FUNCTION

The following form was chosen for the objective function

$$J' = c_D' D + c_B' B - c_F F - c_S S - c_W W - c_E E - I \qquad (1)$$

where c_{index} is a cost or value factor, D is the distillate flowrate, B is the bottom product flowrate, F is the feed rate, S is the flowrate of the heating medium, steam in this case, W is the water flowrate, E is the electricity consumption in the case of vapour recompression, otherwise this term is ignored and I are fixed costs as salaries, overhead costs, etc By using a total mass balance, F can be eliminated As I are fixed costs they do not contribute to the variable operating costs, hence eqn (1) may be reduced to

$$J = c_D D + c_B B - c_S S - c_W W - c_E E \tag{2}$$

where

$$c_D = c'_D - c_F, \quad c_B = c'_B - c_F$$

When considering the third term in the right-hand side of this equation we have to realize that heat is added to the distillation process at two places in the reboiler and in the feed preheater In the design condition the heat flow to the reboiler is much more than a tenfold of the heat flow to the feed preheater But as the temperature level in the column will be a degree of freedom we also have to consider the variation in reboiling costs compared to the variation in feed preheating costs, or

$$V\frac{\delta \Delta H}{\delta T} \text{ vs } Fc_p \tag{3}$$

where V is the vapour flow from the reboiler, $\delta \Delta H/\delta T$ is the variation of the heat of vaporization with temperature and c_p is the specific heat of the feed

In our particular study the first term in eqn (3) was about five times higher than the second term Therefore the costs of feed preheating were ignored and for the third term in eqn (2) the reboiling costs were taken For the conventional single column and the heat integrated two column system electricity costs were ignored, resulting in an objective function

$$J = c_D D + c_B B - c_S S - c_W W \tag{4}$$

For the vapour recompression system there was obviously no contribution of steam and water costs, hence the objective function can be simplified to

$$J = c_D D + c_B B - c_E E \tag{5}$$

3 PROCESS MODELLING

A static process description gives a good starting point for optimization The result of the static optimization can be that either the process should be kept at one or more constraints or at a hill top In the first case it can be shown [5, 6] that also under dynamic conditions optimal operation is close to the constraint

When the optimum lies on a hill top dynamic variations have to be considered But very often the hill top is rather smooth resulting in minor changes in the objective for small dynamic variations This means that a static optimization will give reasonable results From a practical point of view a static optimization is very much preferred over a dynamic optimization of a detailed dynamic model

The static model used in this study is given in Appendix I, where the Edmister model [7, 8] for the distillation process is described briefly together with equations for the compressor, reboiler and condensor

In this section the degrees of freedom for optimization will be analysed for the different configurations The selection of degrees of freedom for static optimization is rather arbitrary

(i) *Conventional distillation column*

There are five degrees of freedom for a given feed, which enters the column under boiling point conditions (see Fig 1) the pressure P, the bottom product flowrate B, the distillate flowrate D, the top reflux ratio R_T and the bottom reflux ratio R_B The bottom reflux ratio can be associated with the steam flow to the reboiler As D and B have to be used for level control, there are three remaining degrees of freedom In this study the top product quality was specified for which R_T was chosen somewhat arbitrarily as manipulated variable Hence for the conventional distillation process the two degrees of freedom were the pressure P and the bottom reflux ratio R_B or vapour flow from the reboiler V

(ii) *The vapour recompression system* (see Fig 2)

Compared to the conventional distillation process there is one extra degree of freedom the pressure after compression However, the reboiler and condensor are not independent As the heat transfer in the reboiler/condensor is described by two equations we have to use two degrees of freedom for manipulation in order to fit these equations This finally leaves one degree of freedom, for which the column pressure P is chosen Shinskey [3] proposes a connection between the compressor outlet and the flash tank (see – – – line in Fig 2) This gives an extra degree of freedom Although this flow may be used for control, start-up or shut-down, it should be made equal to zero for optimal operation and it is therefore not used as degree of freedom in this study A trim reboiler is shown which may be used for start-up

(iii) *The heat integrated two column system* (see Fig 3)

For two independent columns there are eleven degrees of freedom Four levels have to be controlled thus leaving seven degrees of freedom the column pressures, the top and bottom reflux ratios and the ratio of the feed rates However, the columns are integrated by the condensor/reboiler The heat transfer in this heat exchanger is described by two equations In order to fit these equations the bottom reflux ratio of column two and the top reflux ratio of column one are used The composition of the mixture of the distillate flows is specified and the second column top reflux ratio is chosen arbitrarily to meet this specification This finally leaves four degrees of freedom for this system the column pressures P_1 and P_2, the first column bottom reflux ratio R_{B1} and the ratio of the feed rates F_1/F_2

4 LIMITATIONS IN OPERATION

The study on optimal operation would lose its reality when the system constraints were left out of consideration There are four constraints which will be dealt with in some more detail the reboiler constraint, the condensor constraint and the column tray constraints

(i) *The reboiler constraint*

In this case study heat is transferred by condensing steam to the boiling bottom product We are only concerned with the limitation to heat transfer, which is assumed to be reached at the maximum condensing rate of the steam When the steam side is considered isothermal, the driving force for heat transfer is the temperature difference between the steam side and the boiling bottom product When ignoring superheating of the steam, the maximum amount of heat that can be transferred may be described by

$$Q_{R\,\max} = U_R A_R (T_{s\,\max} - T_{\text{bottom}}) \tag{6}$$

where $Q_{R\,\max}$ is the maximum heat transfer in the reboiler, U_R is the overall heat transfer coefficient in the reboiler, A_R is the reboiler area and $T_{s\,\max}$ is the saturated steam temperature at the maximum steam pressure

(ii) *The condensor constraint*

In this study water was used as a cooling medium Its temperature is higher in summer than in winter A rather unfavourable situation was taken a summer inlet water temperature of 293 K The condensor constraint will shift to higher capacities for lower inlet temperatures The maximum amount of heat is transferred when the outlet water temperature approaches the inlet temperature asymptotically

The maximum amount of heat $Q_{c,\max}$ can be calculated from

$$Q_{c\,\max} = U_c A_c (T_{\text{top}} - T_{w\,\text{in}}) \tag{7}$$

where U_c is the overall heat transfer coefficient in the condensor A_c is the condensor heat transfer area

A more accurate but also complicated way of computing maximum loadings is to consider control valves in the supply lines The constraints are reached when the valves are wide open

(iii) *Column constraints*

We shall not consider weeping and pulsation, phenomena which are related to low flows in the column At high liquid and vapour flow flooding becomes a limitation in the operation The most well-known method to predict flooding is a correlation by Fair *et al* [9] For each tray spacing the maximum allowable vapour flow follows from

$$V_{\max} = \left(\frac{\sigma}{0\,02}\right)^{0\,2} \frac{A_d}{M} [\rho_v(\rho_l - \rho_v)]^{0\,5} f\left[\frac{L}{V}\left(\frac{\rho_v}{\rho_l}\right)^{0\,5}\right] \tag{8}$$

where σ is the surface tension, N/m M is the molecular weight, A_d is the column cross sectional area, m^2, ρ is the density, kg/m^3, and f a functional relationship This relationship from Fair's data was approximated by a third order polynomial As conditions are different at every tray, eqn (8) was computed for the top, feed and bottom tray Surface tension and densities were calculated as a function of composition and pressure, using the data given in references [3, 10, 11]

Another column constraint to be considered is the maximum allowable operating pressure The column and vessels are protected from overpressure by relief valves Operating pressure must not be allowed to approach these relief settings

For the propane/propene system a maximum design pressure of 30 bar was used, although in one case a value of 38 bar was used For the butane/isobutane system a maximum design pressure of 15 bar was used

5 COMPUTATIONAL ASPECTS

To optimize the static models the flexible polyhedron search method originally proposed by Nelder and Mead [12] was used Quadratic loss penalty functions [13] were introduced to guard against violation of limitations Top product specification was met by iterating over the top reflux ratio

Convergence of the optimization procedure from different starting points was satisfactory in all cases

6 RESULTS

(i) *Conventional distillation column*

First we shall discuss the operation of separating a propane/propene mixture in the column as shown in Fig 1 There are two degrees for optimization the column pressure P and the vapour flow from the reboiler V The value of the objective function is proportional to the feed flow F, hence it can be plotted in a graph with P and V/F along the axis This is done in Fig 4 For the construction of this figure the values given in Appendix II, Table A, were used The objective function is given in Dfl/kmole feed Plotting all significant constraints in the same figure results in an operating window Boil-up and pressure must be maintained within this window or along any borderline Under changing conditions the constraints will shift At higher feed rates they shift downwards, which means that the reboiler constraint will become critical From Fig 4 it can be seen that the optimum is rather smooth Along the lower part of the contour $J/F = 11\,00$ the value of V/F is approximately constant for values of the pressure between 21 and 30 bar, and deviates only 0 2 per cent from the optimum

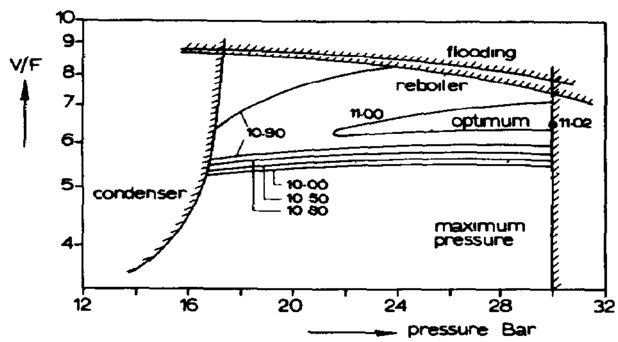

Fig 4 Operating window for the separation of propane/propene

The optima for different feed rates are given in Table 1 V denotes the vapour flow from the reboiler and J/F the value of the objective function per kmole feed It can be seen that as long as the reboiler loading is not maximal the V/F ratio is approximately constant Therefore V and F are controlled in ratio by means of the control valve in the water supply (see Fig 5) The vapour flow is calculated from a heat balance over the water side of the condensor

$$V = \frac{\phi_w C_{pw}(T_{w\,\text{out}} - T_{w\,\text{in}})}{\Delta H_{\text{propene}}} \tag{9}$$

where ϕ_w is the water flow, c_{pw} is the specific heat

Table 1 Optima for distillation of propane/propene in a conventional distillation column

P bar	F kmol/hr	x_B %propene	V/F	V kmol/hr	steam flow kg/hr	J/F Dfl/kmol	constraint
30 0	250	3 45	6 66	1664	8328	11 026	pressure
30 0	300	3 51	6 63	1988	10062	11 019	pressure
27 6	350	3 76	6 37	2229	11703	11 007	reboiler
22 7	400	4 01	5 97	2387	13406	10 978	reboiler

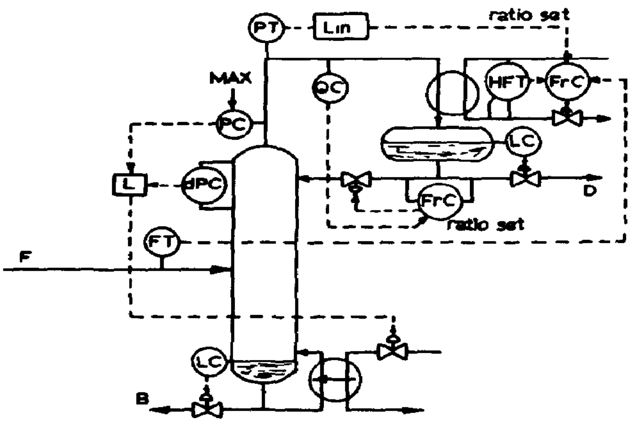

Fig 5 Constraint control scheme for propane/propene distillation in a single column

The top product quality is controlled by the reflux The pressure may then be controlled by the steam flow When the steam valve is wide open, the pressure will decrease as it is desired to manage a higher throughput (see Fig 4) For low pressures the column may be close to the flooding constraint Therefore a differential pressure controller can reduce the steam flow by means of a low value selecting device

When the pressure is decreased the V/F ratio is not constant anymore, but has to be reduced The results of Table 1 may be approximated by the following linear relationship

$$\frac{V}{F} = \alpha P + \beta \tag{10}$$

thus giving the ratio set of the flow ratio controller on the cooling water supply

In a similar way as for the propane/propene distillation, an operating window can be constructed for the separation of butane/isobutane Results are given in Fig 6 The optimum value of the objective function per kmole feed is equal to 6 59 On the condensor constraint, the value of the objective deviates only 0 01 per cent from its optimum for the same (V/F) value For the construction of Fig 6 the values given in Appendix II Table B, were used

The optima for different feed rates are given in Table 2 From Table 2 the locus of optimal operating points may be given by

$$P = \alpha \frac{V}{F} + \beta \tag{11}$$

where α and β are constants

On the basis of Fig 6, Table 2, and eqn (11) the control scheme of Fig 7 may be constructed

(ii) *The vapour recompression system*

As discussed previously, the column pressure P is the only degree of freedom The value of the objective

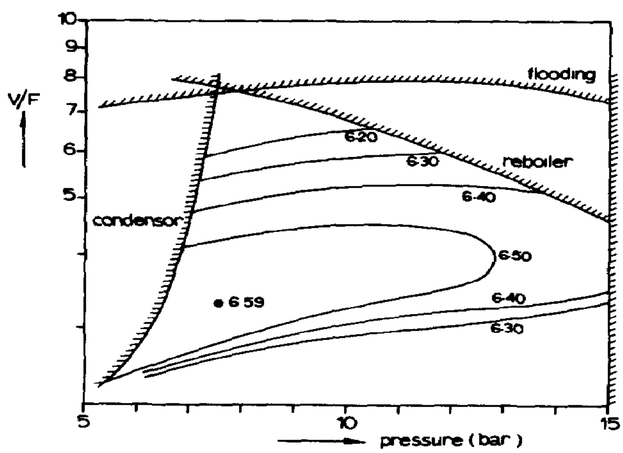

Fig 6 Operating window for the separation of butane/isobutane

Table 2 Optima for distillation of butane/isobutane in a conventional distillation column

P bar	F kmol/hr	x_B % isobutane	V/F	V kmol/hr	steam flow kg/hr	J/F Dfl/kmol	constraint
6 29	350	9 44	3 18	1114	9179	6 623	
6 92	400	10 17	3 25	1301	10686	6 607	
7 52	450	10 83	3 32	1493	12229	6 591	
8 23	500	11 39	3 40	1701	13894	6 573	condensor
8 98	550	11 96	3 49	1918	15624	6 55[illegible]	condensor
9 79	600	12 76	3 57	2140	17366	6 5[illegible]	condensor & reboiler

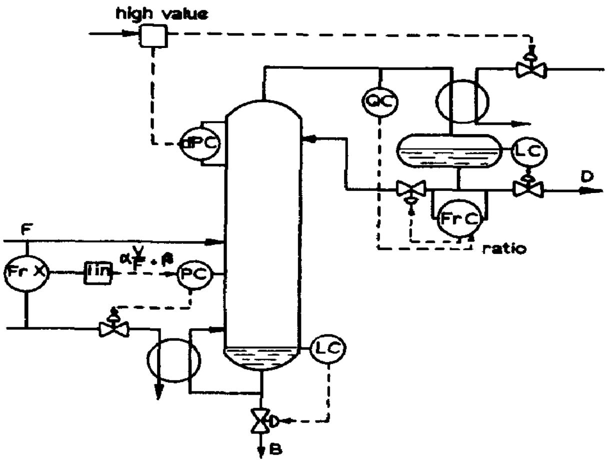

Fig 7 Constraint control scheme for distillation of butane/isobutane

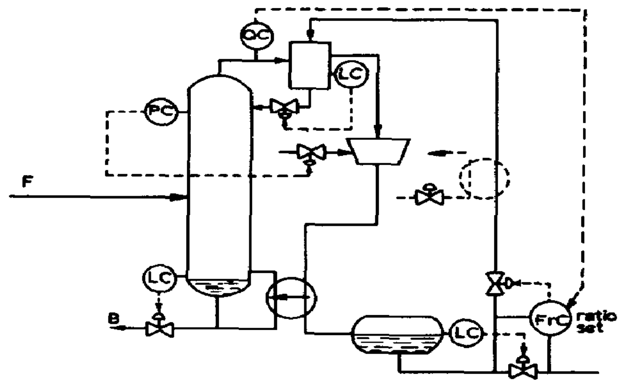

Fig 8 Constraint control scheme for distillation of propane/propene in case of vapour recompression

function for different values of P for the distillation of propane/propene are given in Table 3, for the distillation of butane/isobutane some data are given in Table 4 The modifications of the design data in Appendix II, Table A and B, are given in Table C and D respectively

As can be seen from Table 3 for the propane/propene system, the pressure should be kept more or less at a maximum value However, for the distillation of butane/isobutane the pressure should be kept at a minimum value (Table 4) The control scheme for both systems is given in Fig 8, where the speed of the compressor is controlled by a pressure controller

Shinskey [3] argues that the steady-state effect of compressor speed on the pressure is small, because this is a closed system An increase in speed can reduce suction pressure, increase discharge pressure, and increase flow But the higher flow will increase the rate of heat transfer The higher reboiler-condensate temperature will increase reflux flashing and ultimately raise column pressure

However, when we inspect, for example, the data for the compression of propene vapour, we see that an increase in pressure will reduce the work introduced by

Table 3 Results for propene vapor recompression

F kmol/hr	P bar	P_c bar	R	J/F Dfl/kmol	Electr cons MW
500	6	10 9	7 64	11 38	1 5
500	14	23 1	8 95	11 46	1 1
500	22	32 4	9 85	11 45	1 1
500	30	43 6	10 58	11 48	1 0
600	6	11 9	7 64	11 32	2 2
600	14	24 5	8 96	11 40	1 7
600	22	35 4	9 87	11 38	1 8
600*	26	41 5	10 25	11 44	1 5
700	6	12 3	7 65	11 27	3 0
700	14	27 2	8 98	11 34	2 5
700*	16	30 6	9 23	11 32	2 6

* indicates flooding.

Table 4 Results for isobutane vapour recompression

F kmol/hr	P bar	P_c bar	R	J/F Dfl/kmol	Electr cons MW
450	12 0	21 3	7 42	6 80	1 1
450	8 0	14 7	6 20	6 85	1 2
450	4 0	7 6	4 77	7 00	1 2
450	2 0	3 9	3 84	7 03	1 2

the compressor. This will have a stabilizing effect on the pressure.

If the controlled system could drift to an undesired operating point, installation of a cooler would be necessary. Shinskey [3] proposes a connection between compressor outlet and flash tank. This is a far from optimal solution of the control problem since only part of the heat in the compressed vapour is used for reboiling. Therefore we studied an alternative solution by installing the cooler in the return line from top product accumulator to flash tank. This system has two degrees of freedom for which the column pressure P and the vapour flow through the compressor ϕ_c were selected.

Results for propene compression are given in Fig. 9, for a feedrate of 500 kmoles/hr. It can be seen that the optimum lies on the interconnection of two constraints: the maximum pressure and no cooling constraint. Cooling decreases the value of the objective function but it should be noted that the optimum is rather flat. Results for isobutane compression are given in Fig. 10, for a feedrate of 450 kmoles/hr. It is evident that for the range of parameters investigated pressure should be minimized, resulting in a maximum cooling water flow to the condensor. Pressure can again be controlled by the compressor speed.

(iii) The heat integrated two column system

Two case studies have been made for the distillation of propane/propene. The details of the design of the system for case study one are given in Appendix II, Table E, where only the modifications to Table A are given. The results of this optimization study are given in Table 5;

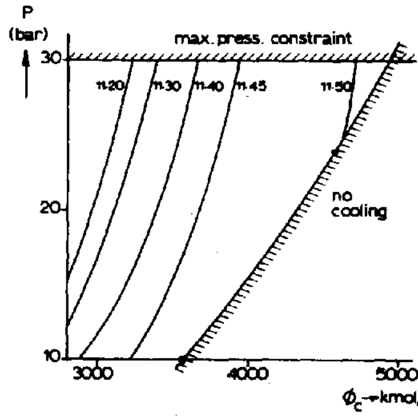

Fig. 9. Value of the objective function vs pressure P and compressor flowrate ϕ_c in case of vapour recompression with cooling.

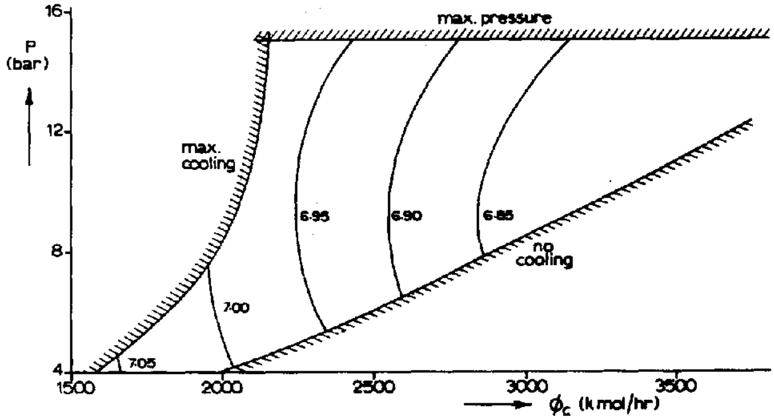

Fig. 10. Value of the objective function vs pressure P and compressor flowrate ϕ_c in case of isobutane vapour recompression with cooling.

Table 5. Optimization of integrated columns, case study one

X_F	F_1 kmol/h	F kmol/h	P_2 bar	R_{T1}	R_{T2}	X_{D1}	X_{D2}	steam cons. 10^{-3} kg/h	J/F Dfl/kmol	Notes
0.6	203.9	600	24.7	28.3	9.6	1.0000	0.9850	7.7	14.32	1,2,4
0.6	266.2	700	24.4	21.4	9.5	0.9999	0.9841	9.6	14.26	1,2,3,4
0.6	300.1	750	24.5	19.1	9.4	0.9998	0.9837	9.6	14.21	1,2,3,4
0.6	162.6	600	24.2	35.4	9.6	1.0000	0.9863	6.8	14.37	1,2,5
0.6	252.2	700	24.2	22.5	9.5	0.9999	0.9845	9.6	14.32	1,2,5
0.5	293.2	750	24.6	19.5	9.5	0.9998	0.9839	9.6	14.27	1,2,3,5
0.5	205.6	600	24.5	33.5	11.3	0.9999	0.9849	8.3	12.89	1,2,4
0.7	183.3	600	24.7	26.9	8.3	1.0000	0.9857	6.8	15.77	1,2,4

notes: 1) bottom of column two on flooding constraint
2) pressure in column one on constraint of 38 bar
3) reboiler constraint
4) water costs 10 cts/m3
5) water costs 2 cts/m3

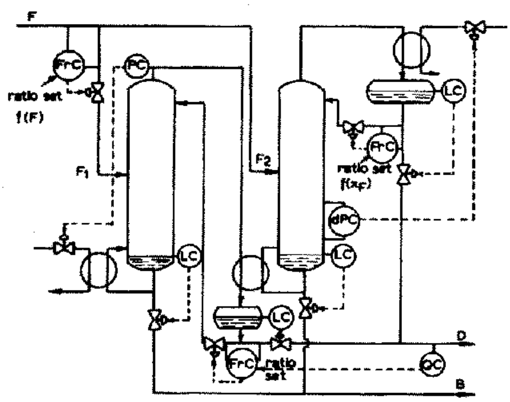

Fig. 11. Constraint control scheme from Table 5.

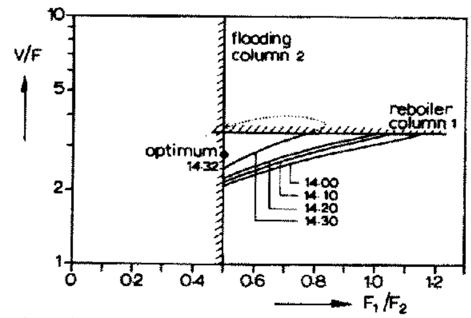

Fig. 12. Value of the objective function for two remaining degrees of freedom.

the constraint control scheme in Fig. 11. As can be seen the first column is on the pressure constraint of 38 bar and the second column is on the flooding constraint. Therefore the pressure has to be maintained on its maximum value, for which the steam flow may be chosen, and the differential pressure, as an indication for the column loading, is maintained on its maximum allowable value by adjusting the cooling water flowrate.

The number of degrees of freedom is now reduced from four to two. The remaining ones can be chosen in different ways. For instance one may choose the ratio of the feed rates and the top reflux ratio of column two. As can be seen from Table 5 the ratio setting of the flow controller of feedrate F_1 mainly depends on the total feedrate, although there is also a dependance on the feed composition and the value of top and bottom product. The ratio setting of the flow controller of the reflux to the second column mainly depends on the feed composition. This composition may be estimated from the ratio of the distillate flow and feed rate.

As also can be seen from Table 5 the pressure in the second column is more or less constant. If both column pressures P_1 and P_2 are fixed on 38 and 24.7 bar respectively we can plot the value of the objective function with the dimensionless vapour flow V/F and the ratio of the feed rates F_1/F_2 along the axis. This is done in Fig. 12. For a one per cent deviation of the optimum profit, V/F may vary with about 15 per cent and F_1/F_2 with about 20 per cent.

For another set of parameters (case study two) given in Appendix II Table F, the system was also optimized. As the column diameters were increased and the pressure constraint decreased, the flooding constraint was not critical anymore. The results are given in Table 6. It can be seen that for a propene feed concentration of 60 mole per cent, the feed is more or less equally distributed between the two columns, while in Table 5 there is a rather asymmetric feed distribution. The control scheme based on Table 6 is given in Fig. 13. As flooding is not critical now the pressure in the second column can be controlled by the cooling water flowrate. When flooding starts, it will be at the bottom of the second column. In that case a differential pressure controller may adjust the cooling water flow rate by means of a high value selector (a higher value reduces cooling water flow).

It should be noted that the top product compositions of both columns are different. Where the first column produces a distillate with very high purity, the second column gives a distillate flow which is less pure. This is due to the fact that the first column is operated under

Table 6. Optimization of integrated columns, case study two

x_F	F_1 kmol/h	F kmol/h	P_2 bar	R_{T1}	R_{T2}	x_{D1}	x_{D2}	steam cons. 10^{-3} kg/h	J/F Dfl/ kmol	notes
0.6	296.6	600	20.34	13.1	9.1	0.9982	0.9822	10.6	11.29	1,3
0.6	364.0	700	20.13	11.1	9.3	0.9937	0.9861	12.1	11.24	1,2,3
0.6	402.8	750	19.83	10.8	9.4	0.9924	0.9873	12.1	11.18	1,2,3
0.6	250.5	600	19.58	18.4	9.1	0.9998	0.9832	9.1	11.35	1,4
0.6	344.2	700	19.64	13.1	9.0	0.9982	0.9823	12.1	11.31	1,2,4
0.6	373.8	750	19.83	11.6	9.1	0.9958	0.9844	12.1	11.28	1,2,4
0.7	251.9	600	20.06	14.2	7.8	0.9998	0.9831	8.7	12.50	1,4
0.5	237.2	600	24.8	10.6	10.6	0.9999	0.9837	9.2	10.23	1,4

Notes: 1) pressure in column one on constraint of 30 bar
2) reboiler constraint
3) water costs 10 cts/m3
4) water costs 2 cts/m3

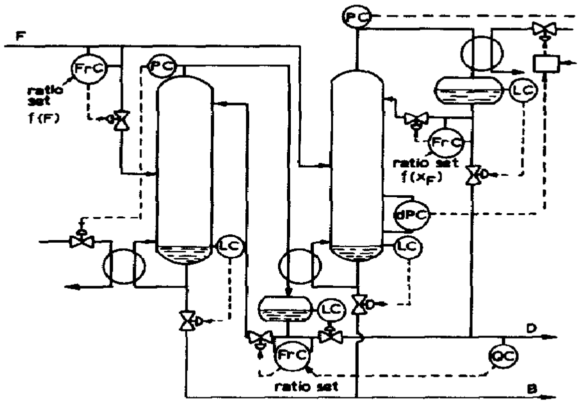

Fig 13 Constraint control scheme from Table 6

high pressure with a resulting low heat of vaporization, high vapour flow and high reflux ratio The second column is operated under lower pressure with a lower reflux ratio

7 DISCUSSION

First the distillation of the propane/propene mixture will be discussed From Table 1 for the conventional distillation process, it can be seen that the pressure should be maximized, and the average value of the objective function is equal to about 11 00 Dfl/kmole feed The average steam costs are between 0 40 and 0 77 Dfl/kmole feed, depending on the operating pressure

When the steam costs are ignored, the pressure tends to go to a minimum since at lower pressure the separation is less difficult When the steam costs are high we have a different situation An increase in column pressure decreases the heat of vaporization of the bottom product, and decreases the costs of heating considerably On the other hand the reflux ratio has to be increased to meet the top product specification, which leads to an increase in heating costs

It depends on the relative magnitudes of these two effects what the pressure will do For the propane/propene system, with the given energy costs, a maximum pressure leads to a higher value of the objective function When the heat of vaporization is taken as a constant, as many authors do, this will almost always lead to minimum pressure operation The same effects play a role in the operation of the two column system, where the pressure is also maximized The average value of the objective function is between 11 25 and 11 30 Dfl/kmole feed, the average steam costs 0 20 to 0 30 Dfl/kmole feed For the compression system the energy costs are mainly the costs of vapour recompression These costs are 0 20–0 43 Dfl/kmole feed and the pressure should be maximized again The value of the objective function is between 11 32 and 11 48 Dfl/kmole feed at the highest allowable pressure

If only operating costs are considered, a vapour recompression system should be preferred for the distillation of propane/propene

The steam savings of a two column system compared to the one column system are worth mentioning These savings are equal to about a factor of two Also in the case of the distillation of butane/isobutane a vapour recompression system gives a higher value of the objective function than a conventional distillation process

When comparing the distillation of the two binary mixtures in a conventional column it can be seen that the pressure tends to go to a maximum for propane/propene whereas for butane/isobutane the pressure tends to go to a minimum Obviously the separation is much easier at low pressure for the last system Therefore a low reflux ratio accounts for higher contribution to the value of the objective function than the extra expenses on steam costs

Tyreus and Luyben [2, 4] also made a study on distillation in a two column system and a vapour recompression system These authors rejected the compression system, because of its high maintenance costs and bad reliability These aspects are left out of consideration in this work

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NOTATION

A	area, m^2
A_i	absorption factor on tray i
B	bottom product flow rate, kmol/hr
C_{index}	cost or value factor, Dfl/kmol
$C_{1\ 5}$	constant
C_p	specific heat, J/kgK
D	distillate flow, kmol/hr
E	electricity consumption, kWh
F	feed rate, kmol/hr
f	fugacity
f_l	liquid part of the feed, kmol/hr
H	enthalpy, J/kmol
ΔH	heat of vaporization, J/kmol
I	fixed costs
J	objective function, Dfl/hr
K	distribution coefficient
L	liquid flow rate, kmol/hr
l	tray liquid flow, kmol/hr
M	molecular weight
P	pressure, bar
P_i^o	pure component vapour pressure, bar
Q	heat flow, kJ/hr
R_T, R_B	top and bottom reflux ratio
S	steam flow, kg/hr
T	temperature, K
U	heat transfer coefficient, W/m^{2}K
V	vapor flow rate, kmol/hr
v	tray vapour flow, kmol/hr
W	water flow rate, kg/hr
x	liquid composition
y	vapour composition
Z_i	parameter defined in (I 9)

Greek symbols

α constant
β constant
ϕ flow rate, kg/hr
ϕ_{Ai} parameter defined in appendix I
ϕ_{si} parameter defined in appendix I
ρ density, kg/m^3
κ ratio of specific heats
σ surface tension, N/m

Indices

B bottom
C condensor
D distillate
E electricity
F feed
l liquid
R reboiler
S steam
v vapour
W water

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APPENDIX I. PROCESS MODELLING

(i) *Edmister model for the distillation column*

In the Edmister model an absorption factor is defined for each component as

$$A_{i,n} = \frac{l_{i,n}}{v_{i,n}} = \frac{L}{V}\ K_{i,n} \tag{I 1}$$

where $l_{i,n}$ is the flow of component i on tray n, $v_{i,n}$ is the vapour flow of component i on tray n, L, V is the average liquid and vapour flow in the absorption section and $K_{i,n}$ is the distribution coefficient of component i on tray n

The distribution coefficient is calculated from

$$K_{i,n} = \left(\frac{f_p p_i^\circ}{f_t p}\right)_n \tag{I 2}$$

where f_p is the fugacity for correction of the vapour pressure, f_t is the fugacity for correction of the total pressure, p_i° the pure component vapour pressure of component i and p is the total pressure

From a mass balance at the top of the column we can derive

$$\frac{L}{V} = \frac{R_T}{1+R_T} \tag{I 3}$$

with R_T the top reflux ratio

Absorption factors are calculated for feed and top tray respectively, denoted with $A_{i,\text{feed}}$ and $A_{i\,\text{top}}$ and averaged

$$\bar{A}_i = \sqrt{A_{i,\text{feed}}(1 + A_{i,\text{top}}) + 1/4} - 1/2 \tag{I 4}$$

In a similar way stripping factors are defined and averaged

$$S_{i,n} = \frac{V}{L}\ K_{i\,n} \tag{I 5}$$

$$\frac{V}{L} = \frac{R_B}{1+R_B} \tag{I 6}$$

with R_B the bottom reflux ratio and

$$\bar{S}_i = \sqrt{S_{i,\text{feed}}(1 + S_{i\,\text{bottom}}) + 1/4} - 1/2 \tag{I 7}$$

From partial and total mass balances it can be derived that

$$B_i = \frac{f_{L,i} - F_i Z_i}{(R_B+1)\phi_{Si} - Z_i} \tag{I 8}$$

in which

$$Z_i = (1+R_T)\left(1 - \phi_{Ai} - \frac{R_T}{1+R_T}\right) \tag{I 9}$$

$$\phi_{Ai} = \frac{1-\bar{A}_i^{n+1}}{1-\bar{A}_i} - \frac{R_T}{1+R_T}\ \frac{1-\bar{A}_i^n}{1-\bar{A}_i} \tag{I 10}$$

$$\phi_{Si} = \frac{1-\bar{S}_i^{m+1}}{1-\bar{S}_i} - \frac{R_B}{1+R_B}\ \frac{1-\bar{S}_i^m}{1-\bar{S}_i} \tag{I 11}$$

$f_{L,i}$ is the liquid fraction of the feed, which is equal to F_i when the feed enters the column at boiling point conditions

The parameters m and n denote the number of trays in the stripping and absorption section The distillate flow follows from

$$D_i = F_i - B_i \tag{I 12}$$

and from summation

$$D = \sum D_i \text{ and } B = \sum B_i \tag{I 13}$$

thus the top vapour concentration of component i is

$$y_{\text{top},i} = \frac{D_i}{D} \tag{I 14}$$

and the bottom liquid concentration

$$x_{\text{bottom},i} = \frac{B_i}{B} \tag{I 15}$$

Calculation procedure

Select the column pressure P, the top reflux ratio R_T and the bottom reflux ratio R_B For given feed composition and pressure the boiling point of the feed can be calculated Select top and bottom temperature equal to the feed temperature

From the Antoine equation the partial vapour pressure of the components can be calculated for a given temperature [10]

This is done for top, feed and bottom tray Together with the activity coefficients taken from literature [12, 13] the distribution coefficient can be calculated according to eqn (I 2)

With the aid of (I 1) and (I 3)–(I 13) top and bottom product compositions can be calculated From these bubble and dewpoint temperatures can be computed by means of the two following equations

$$\left(\sum_i \frac{x_i \gamma_i p_i^o}{P}\right)_{\text{bottom}} = 1 \tag{I 16}$$

and

$$\left(\sum_i \frac{Y_i P}{\gamma_i p_i^o}\right)_{\text{top}} = 1 \tag{I 17}$$

The calculations are repeated using the last two temperatures as bottom and top temperature respectively, until the difference between the two pairs of temperatures is sufficiently small

(ii) *Reboiler*

In the Edmister model the vapour flows are calculated as well as the temperatures For a given temperature the heat of vapourization can be calculated, resulting in a value of the heat to be transferred Q_R The steam temperature is then computed from

$$T_{\text{steam}} = T_{\text{bottom}} + \frac{Q_R}{U_R A_R} \tag{I 18}$$

At this steam temperature the heat of condensation is ΔH_{steam} The steam flow can now be calculated from

$$\phi_{\text{steam}} = \frac{Q_R}{\Delta H_{\text{steam}}} \tag{I 19}$$

(iii) *Condensor*

At a given column top temperature the heat of condensation can be calculated, resulting in a value of the heat to be transferred Q_c The cooling water outlet temperature is calculated from

$$T_{w,\text{out}} = T_{\text{top}} - (T_{\text{top}} - T_{w,\text{in}}) e^{[U_c A_c / Q_c](T_{w,\text{in}} - T_{w,\text{out}})} \tag{I 20}$$

and the waterflow from

$$\phi_{\text{water}} = \frac{Q_c}{c_{pw}(T_{w\,\text{out}} - T_{w\,\text{in}})} \tag{I 21}$$

(iv) *Integrated reboiler/condensor*

Equations are given for the reboiler/condensor of the two column system For the vapour recompression system similar equations hold Equation (I 22) has only to be extended with a term due to superheating The two heat transfer equations are

$$V_{\text{top}\,1}\ \Delta H_{\text{top}\,1} = V_{\text{bottom}\,2}\ \Delta H_{\text{bottom}\,2} \tag{I 22}$$

and

$$Q_{R\,c} = U_R A_R (T_{\text{top}\,1} - T_{\text{bottom}\,2}) \tag{I 23}$$

(v) *Compression*

For polytropic compression the following relationship holds

$$P_c = P_{\text{top}} \left(\frac{T_c}{T_{\text{top}}}\right)^{\mu/(\mu-1)} \tag{I 24}$$

with $\mu > \kappa$, and κ being the ratio of specific heats The index c denotes the discharge conditions The energy consumption can be determined from the enthalpy difference between compressor inlet and outlet The enthalpy is determined from

$$H_i = C_1 T_i + C_2 T_i^2 + C_3 P_i + C_4 P_i^2 + C_5 P_i T_i \tag{I 25}$$

where C_1 to C_5 are constants

(vi) *Flash tank*

As the pressure in the reboiler is higher than in the flash tank, part of the liquid will evaporate This amount can roughly be calculated from

$$\alpha = \frac{C_p (T_R - T_{\text{top}})}{\Delta H} \tag{I 26}$$

α is the vapour fraction, C_p is the specific heat and T_R is the reboiler temperature

APPENDIX II

Table A Data for the determination of an operating window for the distillation of a propane/propene mixture in a conventional distillation column

Column diameter	2 40 m
Tray spacing	0 6 m
Reboiler area	125 m^2
Condensor area	725 m^2
Feedrate	300 kmoles/hr
Feed composition, propene	0 60
Value distillate	0 385 Dfl/kg
Value bottom product	0 114 Dfl/kg
Steam costs	0 0175 Dfl/kg
Water costs	0 00002 Dfl/kg
Number of trays	180
Feedtray location (bottom = 1)	60
Distillate composition, propene	0 99
Activity coefficients	
Propane, top/feed/bottom	1 0000/0 9997/1 0100
Propene, top/feed/bottom	1 0191/1 0291/1 0051
Overall heat transfer coefficients	
Reboiler	800 kcal/m^2hrK
Condensor	400 kcal/m^2hrK
Pressure constraint	30 bar

Table B Data for the determination of an operating window for the distillation of a butane/isobutane mixture in a conventional distillation column

Column diameter	3 25 m
Tray spacing	0 6 m
Reboiler area	300 m^2
Condensor area	550 m^2
Feedrate	450 kmoles/hr
Feedcomposition, isobutane	0 6
Value distillate	0.140 Dfl/kg
Value bottomproduct	0.100 Dfl/kg
Steam costs	0 0175 Dfl/kg
Water costs	0 00002 Dfl/kg
Number of trays	100
Feedtray location (bottom = 1)	40
Distillate composition, isobutane	0 99
Activity coefficients	1 0000
Overall heat transfer coefficients	
Reboiler	800 kcal/m^2hrK
Condensor	400 kcal/m^2hrK
Pressure constraint	15 bar

Table C Modifications to table A for propene vapour recompression

Column diameter	3.25 m
Reboiler area	800 m^2
Overall heat transfer coefficient	
reboiler/condensor	600 kcal/m^2hrK
Electricity costs	0.10 Dfl/kWh
No condensor	
Feedrate	500 kmoles/hr

Table D Modifications to table B for isobutane vapour recompression

Column diameter	3 75 m
Reboiler area	670 m^2
Overall heat transfer coefficient	
reboiler/condensor	600 kcal/m^2hrK
Electricity costs	0 10 Dfl/kWh
No condensor	

Table E Modifications to table A for the two column system, case study one

Diameter column 1	2 75 m
Diameter column 2	2 40 m
Reboiler area column 1	130 m^2
Reboiler/condensor area	1022 m^2
Condensor area column 2	705 m^2
U condensor/reboiler	600 kcal/m^2hrK
Value distillate	0 485 Dfl/kg
Value bottom product	0 140 Dfl/kg
Water costs	0 00002 or 0 0001 Dfl/kg
Pressure constraint	38 bar
Total feed rate	600 - 750 kmoles/hr

Table F Modifications to table A for the two column system, case study two

Diameter column 1	2.75 m
Diameter column 2	2 40 m
Reboiler area column 1	130 m^2
Reboiler/condensor area	1022 m^2
Condensor area column 2	705 m^2
U condensor/reboiler	600 kcal/m^2hrK
Value distillate	0 485 Dfl/kg
Value bottom product	0 140 Dfl/kg
Water costs	0 00002 or 0 0001 Dfl/kg
Pressure constraint	38 bar
Total feed rate	600 - 750 kmoles/hr