Distillation with Secondary Reflux and Vaporization: A Comparative Evaluation

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A novel distillation scheme which makes use of secondary reflux and vaporization to enhance thermal efficiency is presented. Low operating temperatures, close boiling mixture, and tight product specifications appear to favor this scheme over the conventional distillation. Computer simulation indicates a potential utility reduction of 50 to 75%.

SCOPE

Distillation is the single most important separation unit operation in the process industry. It is widely used to upgrade feedstocks, separate reaction intermediates, and purify products in processes ranging from cryogenic separation of oxygen, nitrogen, and helium to the recovery of aromatics from coal tar. In a recent study carried out under the auspices of the Governor's Energy Advisory Council of Texas, the energy usage of some forty-five refineries (in thirty-nine companies) and 226 chemical plants (in 140 companies) was surveyed (Prengle et al., 1974), and distillation was an important energy consumer in almost all of them. In petroleum refineries which are the largest energy consumers on a per plant basis (1.9×10^{16} J/plant), crude and vacuum distillation alone accounts for 22.5 to 51% of the total energy consumption. Any enhancement of efficiency of this important unit operation could have an impact which will significantly benefit a wide cross section of process industries.

In the conventional distillation column, heat is supplied to the reboiler and removed from the condenser. Because of the temperature difference between the reboiler and the condenser, the separation of components is always accompanied by a degradation of energy, even when heat leaks and other losses are excluded. When we view it as a thermodynamic process, conventional distillation is not particularly noted for its efficiency. Estimates as low as 1.9% have been reported for the thermodynamic efficiency of industrial distillation columns (Freshwater, 1951). It is the confrontation with real processes of such dismal inefficiency that have caused investigators for several decades past to speculate the potential for radical improvement (Freshwater, 1951; Haselden, 1958).

The virtues of the traditional distillation column are its mechanical simplicity and relatively low capital investment. Because energy supplies from fossil fuels (notably, natural gas and petroleum) have been both cheap and plentiful, it was very hard to justify additional equipment and fabrication costs associated with energy efficiency enhancement. But the energy situation has undergone drastic changes in the last few years with costs going up from about 20¢/billion J to as much as \$3/billion J. Schemes for enhancing distillation column efficiency and alternative low energy separation techniques which formerly could be dismissed summarily on economic ground now deserve careful investigation in the new economic circumstances. In a recent NSF conference on "Innovative Design Techniques for Energy Efficient Processes" (Mah, 1975), much time and attention were devoted to the improved design of distillation schemes and the development of new low energy separation techniques.

In this paper we shall present a new distillation scheme which makes use of secondary reflux and vaporization (SRV) to enhance its thermal efficiency. We shall compare its performance quantitatively with an equivalent conventional distillation column. This evaluation is carried out using computer simulations of realistic physical systems. We shall discuss the basis of this comparison and factors influencing the selection of bench mark problems. Finally, we shall discuss our findings and conclusions.

CONCLUSIONS AND SIGNIFICANCE

The evaluation reported in this paper was carried out with reference to light hydrocarbon mixtures. Realistic representation of thermophysical properties was obtained using the Soave-Redlich-Kwong equation of state. The use of a single equation of state was particularly convenient, since enthalpy and entropy values were also required in compression and expansion computation. A modified Wang-Henke method was used to simulate the conventional and the SRV (secondary reflux and vaporization) distillation systems. To provide a realistic basis of comparison, all compression work and energy transfers were converted into equivalent steam and cooling water consumptions. For this purpose, 3.55×10^6 N/m^2 (500 lb/in.^{2} gauge) steam and 294.26°K (70°F) cooling water were chosen as references.

Our investigation shows that for the cryogenic separation of close boiling mixtures, substantial reductions (50 to 75%) in steam and cooling water consumptions could be obtained with the SRV distillation. The single most important factor in the comparison appears to be the temperature range; the SRV distillation is favored at low operating temperatures. Close boiling mixtures and tight specifications also favor its selection over the conventional distillation. Further investigation is underway to delineate the favorable operating regions for the SRV distillation of multicomponent mixtures and to explore the requirements of its physical realization.

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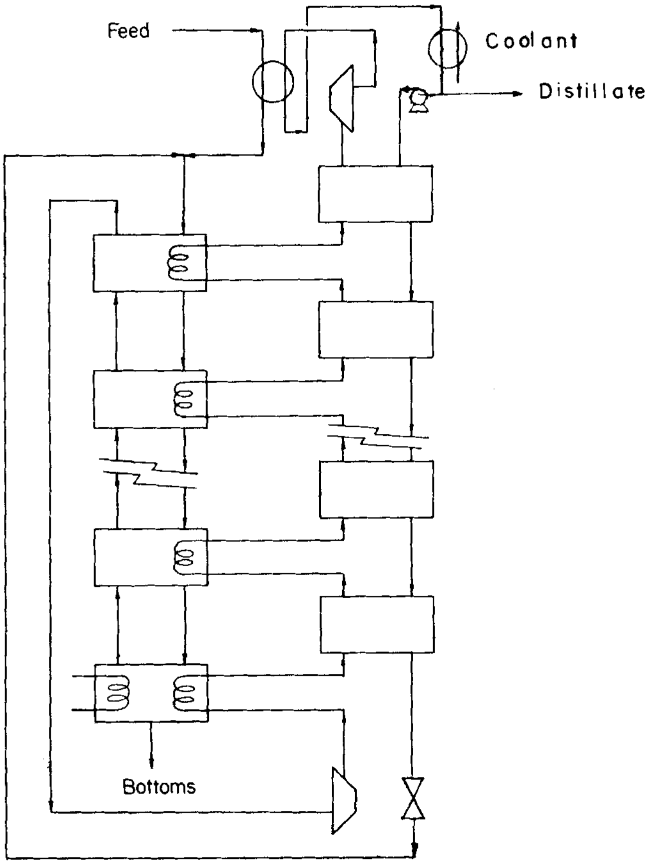

Fig. 1. Distillation with secondary reflux and vaporization

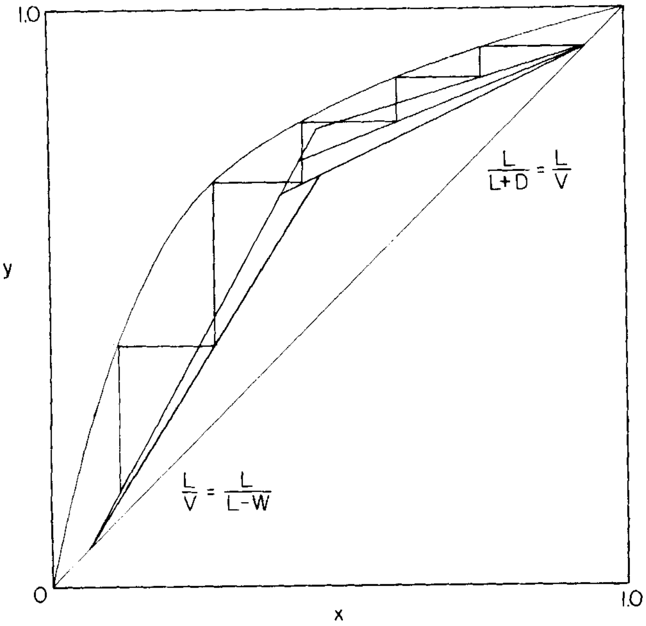

Fig. 2. Modification of operating lines in SRV distillation.

REVIEW OF RELEVANT WORK

In a paper written over a quarter of a century ago, D. C. Freshwater (1951) gave an interesting classification of the various methods for improving the thermal efficiency of distillation equipment. He classified them under three broad headings: multiple effect methods, vapor recompression or heat pump methods, and indirect methods. Most methods fall under the first two categories.

The basic idea of multiple effect methods is to utilize the heat content of the distillate vapor generated in one column to supply the heat required in the reboiler of the next column. Several such schemes are presented and discussed by Robinson and Gilliland (1950). More than one distillation column is involved in the application of these methods.

In order to provide the necessary temperature difference, the columns must be operated under different pressures. In principle, the heat required is reduced roughly by a factor equal to the number of columns employed, if the relative volatility does not change with pressure. However, the heat transfer surfaces required will be larger because of the smaller temperature driving forces. Several of the more elaborate schemes (Guillaume, Mariller, 1943) also fall under this category.

As an alternative to the conventional column design in which heat transfer takes place across solid boundaries in condensers and reboilers, the heat flux can also be utilized for more than one fractionation by the direct contact of vapor and liquid. The so-called thermally coupled distillation was first patented by Brugma in 1937, but interest in this scheme has been revived as a result of several publications in recent years (Petlyuk et al., 1965*a*, *b*, 1966; Stupin and Lockhart, 1972) of which Stupin and Lockhart gave by far the clearest exposition.

In contrast to the multiple effect methods, vapor recompression has been primarily a method of enhancing thermal economy within a single column. Instead of improving efficiency through controlled degradation of energy in stages as in multiple effect methods, vapor recompression attacks the problem at the source. Energy is supplied as the work needed to overcome the thermodynamic irreversibility. Vapor recompression is also discussed in Robinson and Gilliland's book (1950). The great disadvantage of this scheme is that it requires the heat pump to operate over the maximum temperature difference that exists in the system. This is not only thermodynamically less efficient, but it also imposes serious practical limitations on the application of this technique. It is precisely to overcome this difficulty that Freshwater (1961) proposed that the heat pump be applied across a pinch zone over a narrower temperature range. Preliminary evaluation indicates that this modification could give rise to very worthwhile improvement with much less mechanical complications.

SRV DISTILLATION

In contrast to the modifications using multiple effect or vapor recompression in which the internal vapor and liquid traffic remain unaltered, in SRV (secondary reflux and vaporization) distillation the reflux and vaporization rates are deliberately manipulated to enhance the overall thermal efficiency. The manipulation is accomplished through heat exchange between the rectifying and the stripping sections. In order to provide the necessary temperature driving force for the heat to be transferred from the rectifying section to the stripping section, the former must be operated at a higher pressure than the latter. However, in contrast to the vapor recompression scheme, it will not be necessary to apply the compression across the whole temperature span of the column. Moreover, the power expended may be partially recovered through an expander-compressor coupling, although for the purpose of comparative evaluation in this paper no power recovery will be assumed.

Figure 1 shows one such scheme selected for evaluation in this paper. In this scheme the liquid reflux rate steadily increases as we proceed down the rectifying section, and the vapor flow rate steadily increases as we proceed up the stripping section as a result of the heat exchanges between the two sections. Besides the obvious effect of reducing reboiler and condenser duties, the introduction of secondary reflux and vaporization also modify the operating lines. The salutary effect is most easily visualized in terms of a McCabe-Thiele diagram (Figure 2) which shows two families of operating lines corresponding to the conditions of increasing reflux and decreasing vaporization as we proceed down the column. The net effect on the separation is the same as if the operating lines are replaced by a curved operating line which bends away from the vapor-liquid equilibrium line with the result that either fewer stages are needed to accomplish the same separation or better separation is obtained with the same number of stages at the same reboiler and condenser duties. In this illustration we have ignored the effect of pressure on the equilibrium line. In reality, there will be a discontinuity in the equilibrium line due to the fact that the rectifying section is operated at a higher pressure than the stripping section.

BASIS OF COMPARISON

For the purpose of our simulation, the model of a distillation column with equilibrium stages of 100% efficiency is assumed. The governing equations are:

Component material balance for component i on stage j

$$L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} - (W_j + V_j)y_{ij} - (U_j + L_j)x_{ij} + F_{ij} = 0 \quad (1)$$

Phase equilibrium relationship for component i on stage j

$$y_{ij} - K_{ij}x_{ij} = 0 \quad (2)$$

Normalization for vapor mole fractions on stage j

$$\sum_{i=1}^{I} y_{ij} - 1 = 0 \quad (3)$$

Enthalpy balance for stage j

$$V_{j+1}H_{j+1} + L_{j-1}h_{j-1} - (W_j + V_j)H_j - (U_j + L_j)h_j + F_jh_{Fj} - Q_j = 0 \quad (4)$$

and the overall material balance for the rectifying section including stage j

$$\sum_{k=2}^{j} (W_k + U_k - F_k) + L_j - V_{j+1} + d = 0 \quad (5a)$$

or the overall material balance for the stripping section including stage j

$$\sum_{k=j}^{n-1} (W_k + U_k - F_k) - L_{j-1} + V_j + b = 0 \quad (5b)$$

For conventional distillation, the feed, the products, the sidestreams, and the heat removal (F_j, h_{Fj}, b, d, W_j, U_j, Q_j) are specified, and the $(2I + 3)$ equations are used to solve for the $(2I + 3)$ unknowns, x_i, y_i, T, L, and V on each stage. A modified Wang-Henke method (Wang and Henke, 1966; Seader, 1973) was used to solve these equations. The modification provides for the use of the Soave-Redlich-Kwong equation of state to compute the vaporization equilibrium ratio K and vapor and liquid enthalpies H and h.

For SRV distillation, Equations (1) to (5) must be augmented with the additional equations of heat transfer, compression, and expansion. For heat transfer, an overall heat transfer coefficient of 567.8 J/m^2 · s · °K (100 Btu/ft^2-hr-°F) was assumed using the following equation:

$$Q = U_{ov}A\,\Delta T \quad (6)$$

where ΔT is the temperature difference between the paired stages. The compression is assumed to be isentropic, and the expansion is assumed to be isenthalpic. The corresponding equations in terms of the Soave-Redlich-Kwong equation of state are given in Wodnik's thesis (1976).

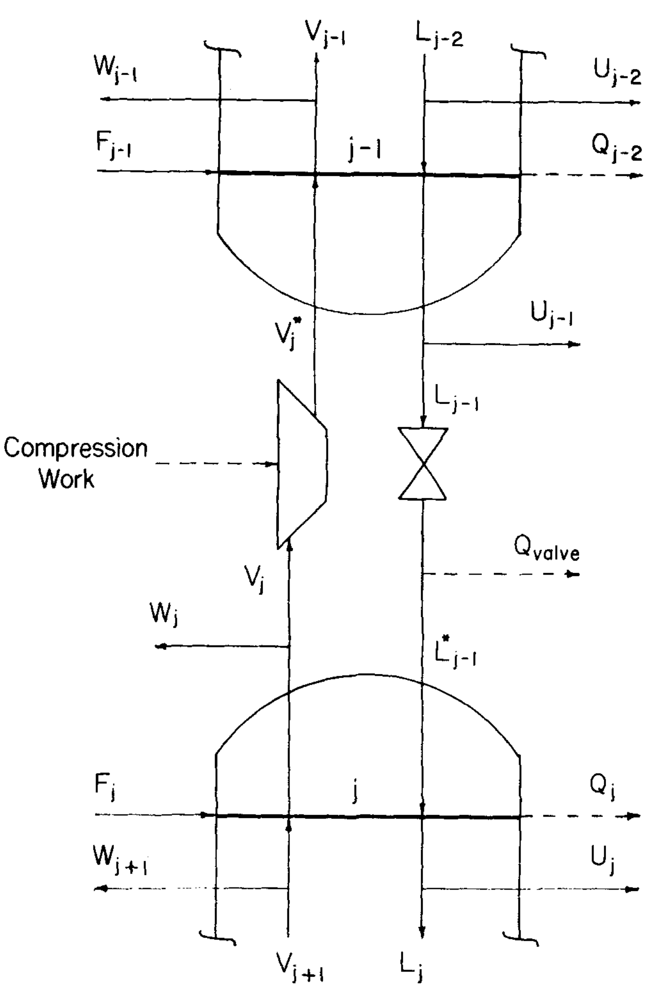

Fig. 3. Schematic representation of the interface between rectifying section and stripping section.

In simulating the SRV distillation we also had to modify the enthalpy balance, Equation (4), for the last stage of the rectifying section and the first stage of the stripping section. With reference to Figure 3, these stages are labeled $(j - 1)$ and j, respectively. For the enthalpy balance around stage $(j - 1)$, the term V_jH_j should be replaced by $V_jH_j^*$, where H_j^* is the enthalpy of the vapor after compression to the prescribed pressure of the rectifying section. Care must be exercised to ascertain that the stream remains completely vaporized by checking the temperature against the dew point temperature. In all instances that we have encountered, the stream was above the dew point temperature. For the enthalpy balance around stage j, the term $L_{j-1}h_{j-1}$ should be replaced by $L_{j-1}h^*_{j-1}$, where h^*_{j-1} is the enthalpy of the liquid at the bubble point temperature corresponding to the stripping section pressure, that is, after the expansion. Normally, the liquid reflux will be a two-phase mixture after the expansion. In order to simplify the computation, it is assumed that this mixture will be cooled until it reaches the bubble point temperature. The cooling or refrigeration required will be referred to as valve cooling in Tables 3 and 6. As we shall see later, this simplification will result in a more conservative evaluation of the performance of SRV distillation.

In the SRV distillation simulation, the column conditions are first initialized without interstage heat transfers. Starting with assumed temperature and vapor flow profiles, the iteration continues until

$$\frac{1}{n}\sum_{j=1}^{n}\left|\sum_{i=1}^{I} x_{ij}-1\right| < 0.025 \qquad (7)$$

At this point heat transfers between paired stages in the rectifying and stripping sections are introduced into the iterative computation. At each macroiteration a modified Wang-Henke method is applied, and compression, expansion, and heat transfer are recalculated. The iteration is terminated when

$$\frac{1}{n}\sum_{j=1}^{n}\left|\sum_{i=1}^{I} x_{ij}-1\right| < 0.001 \qquad (8)$$

In the original Wang-Henke method (Wang and Henke, 1966; Seader, 1973), K values and enthalpies were correlated as polynomial functions of temperature. These representations are not very accurate and reliable, particularly as we lower the temperature and increase the pressure of the mixture. Moreover, the procedure does not lend itself readily to other types of calculations such as compression or expansion. A number of alternatives were considered. The use of a single equation of state to represent both vapor and liquid phases offers considerable flexibility and permits K values, enthalpies, and entropies to be generated on a consistent and unified basis. The best choice based on accuracy, simplicity, and range of applicability seems to be the Soave-Redlich-Kwong equation of state (Soave, 1972). West and Erbar (1973) evaluated four competitive equations of state (BWR-Starling-Han, Lee-Erbar-Edmister, Robinson-Chao, and Soave-Redlich-Kwong) and concluded, "Of these four methods, the Soave-Redlich-Kwong method appears to give the most reliable results for K values, enthalpy departures, and entropy departures over the broadest range of temperature and pressure conditions." Their evaluation was based on the prediction of the thermodynamic properties of light hydrocarbon mixtures which are the systems selected in our studies.

We shall now turn to the comparative evaluation of conventional and SRV distillation. It seems obvious that the two systems should meet the same product specifications in the separation of a given mixture. It is convenient to specify the same number of stages in both systems but to adjust the reflux ratios until the product specifications are just met. But what should the basis of comparison be? A mere summation of reboiler, condenser, and compressor duties would be very misleading, for it does not distinguish energy at different temperature levels. Nor does it recognize the all important difference between heat and work. A comparison based on economic analysis, on the other hand, turns out to be not very practical. The physical realization of the SRV distillation will certainly involve some novel fabrication and configuration, if not equipment. The approximate cost using the Lang factor and proration is insufficiently discerning for a meaningful comparison.

The basis which we finally adopted for this comparison was to convert all quantities in terms of steam at 3.55 × 10^6 N/m^2 and cooling water at 294.26°K. All mechanical work will be converted into steam equivalent by assuming that saturated steam at 3.55 × 10^6 N/m^2 will be expanded in a turbine to the atmospheric pressure. All refrigeration required will be first converted into work equivalent using a specific refrigerant and then converted into steam equivalent as outlined above. In all instances reported in this paper, it is assumed that the refrigerant will reject heat to the cooling water at 299.82°K. A temperature rise of 8.33°K is allowed for the cooling water. Finally, in all instances in which cooling is required, a temperature approach of 5.56°K is assumed between the coolant and the stream to be cooled.

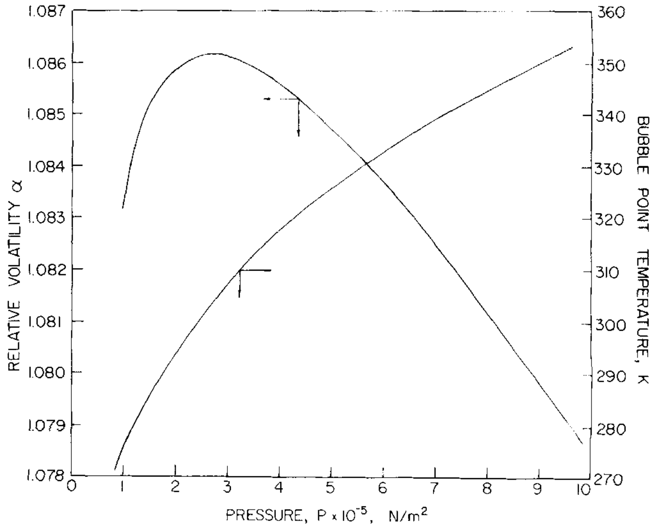

Fig. 4. Effect of pressure on relative volatility and bubble point temperature of an equimolal mixture of trans-2-butene and cis-2-butene.

AREAS OF INVESTIGATION

Before we carry out any quantitative comparison between conventional and SRV distillation, let us consider qualitatively the factors affecting the relative merits of these two schemes. For the same throughput and product specifications, the condenser and reboiler duties are smaller for SRV distillation than for conventional distillation. On the other hand, additional work is required in SRV distillation to compress the vapor from the stripping section to the rectifying section. Since there is a trade off between compression work and thermal energy, neither of these two schemes will be superior over the other under all circumstances. In this evaluation we are interested in delineating circumstances which will favor SRV distillation over conventional distillation and in quantifying the performance difference of these two schemes. What then are those circumstances?

First, any process condition which makes compression work less expensive in comparison with thermal energy tends to favor SRV distillation over conventional distillation. For example, if the distillation is to be carried out at sufficiently low temperatures that refrigeration is required, then the reduction of condenser duty becomes much more significant in comparison with vapor compression. A special

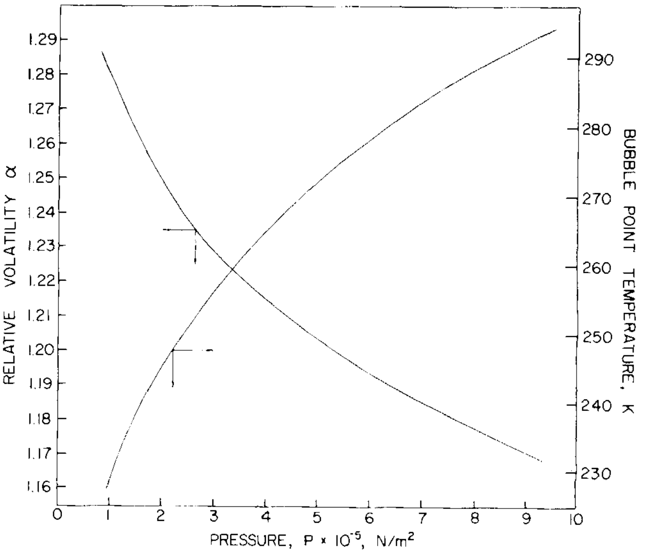

Fig. 5. Effect of pressure on relative volatility and bubble point temperature of an equimolal mixture of propylene and propane.

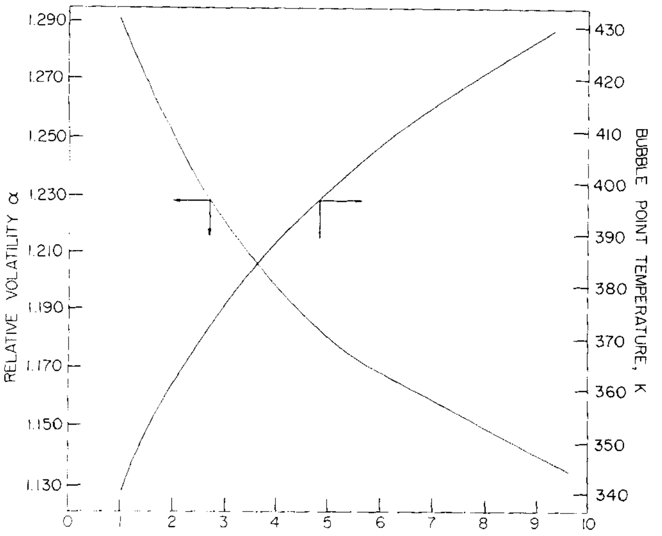

Fig. 6. Effect of pressure on relative volatility and bubble point temperature of an equimolal mixture of 2-methyl pentane and hexane.

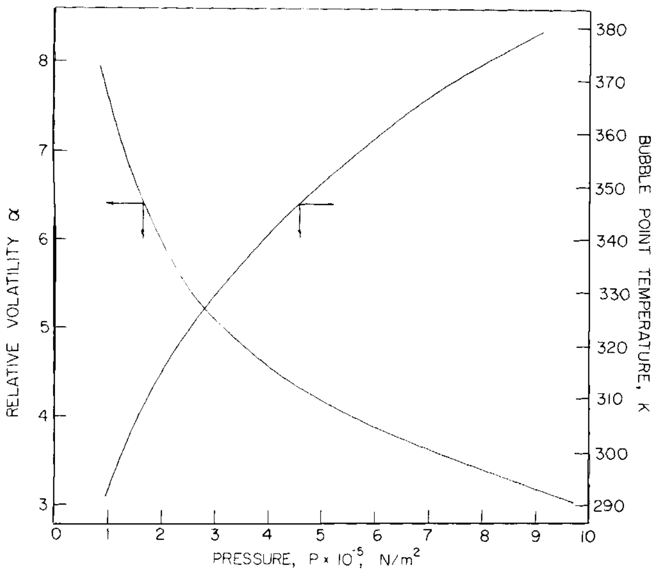

Fig. 8. Effect of pressure on relative volatility and bubble point temperature of an equimolal mixture of cis-2-butene and 2-methyl-pentane.

situation in this category occurs when the distillate temperature is slightly subambient for the conventional column which therefore requires refrigerant cooling. But because of the higher rectifier pressure, the condenser in the SRV distillation may be adequately serviced with cooling water.

Secondly, if the mixture is close boiling, the temperature range between the two ends of the column is smaller, and less compression is needed to reverse the temperature difference between the rectifying section and the stripping section. Also, mixtures whose bubble points increase rapidly with pressure should require less vapor compression to accomplish the same purpose. As a rule, the relative volatility decreases as the pressure is increased and the separation becomes more difficult. This effect tends to work against SRV and multiple effect distillation. Hence, SRV distillation tends to do better for mixtures which do not become much more difficult to separate as the pressure increases.

Thirdly, intuitive reasoning based on the modification of operating lines of the binary system suggests that the SRV distillation will show its best advantages when the separation is difficult and when the operating lines are very close of the equilibrium line. Once again, narrow boiling mixtures seem to fulfill this requirement. But in addition we note that tight product specifications (high purity products) also promote the required circumstance.

The first set of factors discussed above circumscribes the operating conditions, the second set prescribes the selection of the mixture, and the third set points to the product specifications. Based on these considerations, the bench mark problems were selected, and comparative evaluations were made.

DISCUSSION OF RESULTS

The effect of pressure on the relative volatility and the bubble point temperature of different hydrocarbon mixtures was investigated and the results are summarized in Figures 4 to 9 and Table 1. For the purpose of this investigation, binary systems consisting of equimolal mixtures of ethylene, ethane, propylene, propane, trans-2-butene, cis-2-butene, 2-methyl pentane, and *n*-hexane were used and their properties were computed using the Soave-Redlich-Kwong equation of state. The results exhibit several interesting features as noted below:

1. With the exception of the butene mixture in the pressure range 1 to 3 × 10^5 N/m^2, the relative volatility decreases as pressure increases.

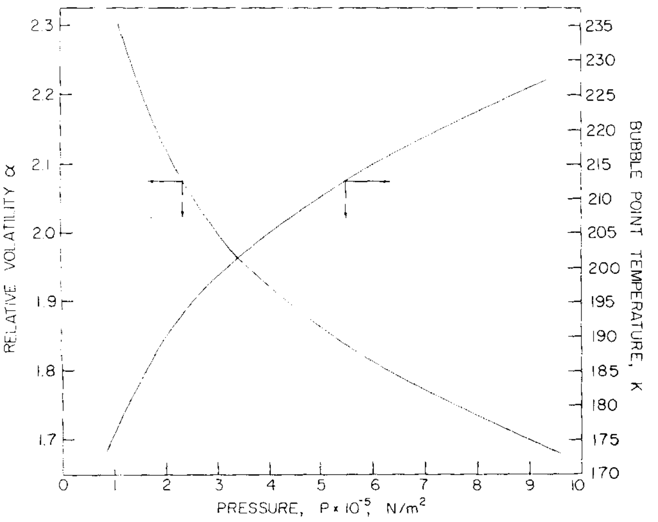

Fig. 7. Effect of pressure on relative volatility and bubble point temperature of an equimolal mixture of ethylene and ethane.

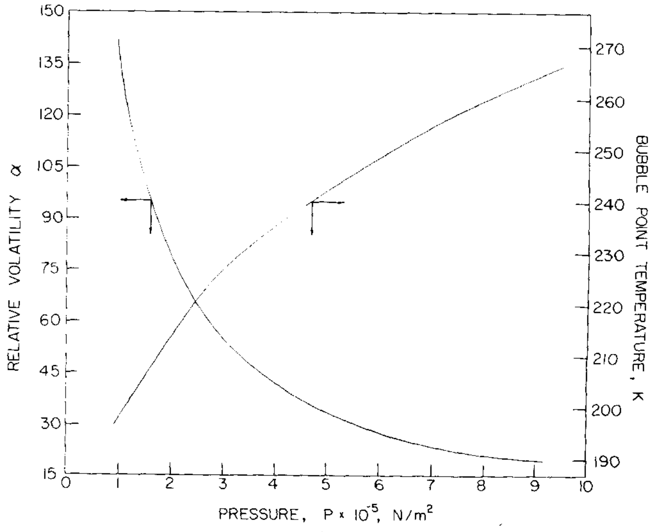

Fig. 9. Effect of pressure on relative volatility and bubble point temperature of an equimolal mixture of ethane and trans-2-butene.

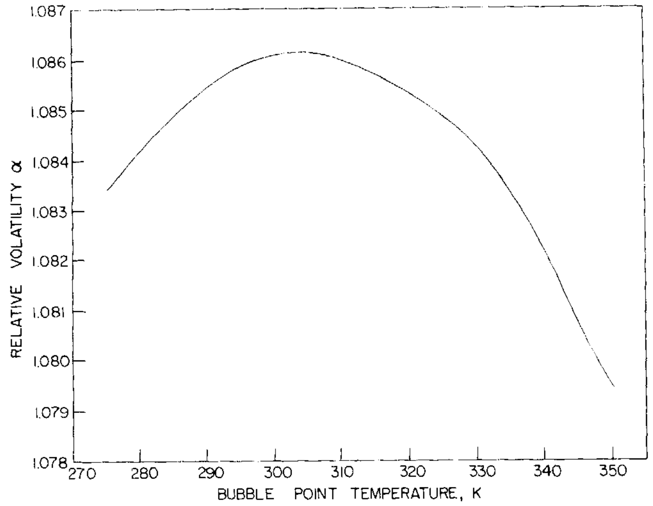

Fig. 10. Relative volatility and bubble point temperature of trans-2-butene and cis-2-butene.

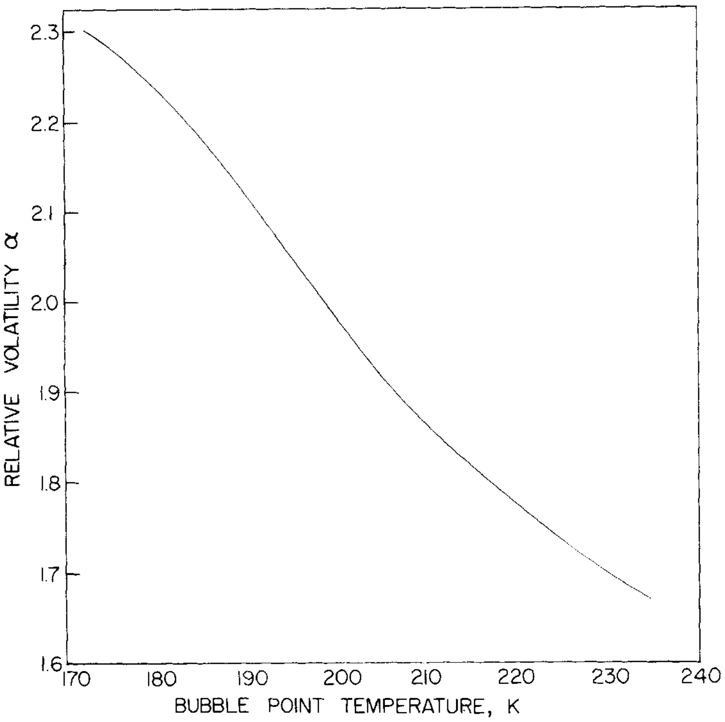

Fig. 11. Relative volatility and bubble point temperature of ethylene and ethane.

2. $d\alpha/dp$ measures the change of relative volatility with pressure. But in order to compare the behaviors of different mixtures, we need to normalize this derivative. Since a relative volatility of one implies no separation, $(\alpha - 1)$ is a measure of separability of the two components, and $d/dp\ \{\alpha/(\alpha - 1)\}$ gives a measure of change of relative volatility with pressure for different mixtures. These values are tabulated in Table 1. We note that at a given pressure $d/dp\ \{\alpha/(\alpha - 1)\}$ is least negative for the closest boiling mixture. As the pressure increases, $d/dp\ \{\alpha/(\alpha - 1)\}$ generally increases, the exception being the cis-2-butene/trans-2-butene mixture.

3. The rate of change of bubble point temperature with pressure decreases as the pressure is raised.

From the viewpoint of selecting bench mark mixtures and operating conditions, it is convenient to plot the relative volatility against the bubble point temperature as in Figures 10 and 11. Over a sufficiently wide range of conditions, the curves appear to be sigmoidally shaped. All other considerations being equal, the desired operating range corresponds to the region in which the relative volatility changes very little for a large change in bubble point temperature. These considerations guided the selection of mixtures and operating conditions used in the following evaluations.

TABLE 1. EFFECT OF PRESSURE ON THE RATE OF CHANGE OF RELATIVE VOLATILITY, $d/dp\ \{\alpha/(\alpha - 1)\}$

Systems	$\frac{d}{dp}\left(\frac{\alpha}{\alpha-1}\right) \times 10^5$, m²/N $P = 1.01 \times 10^5$ N/m²	 $P = 3.04 \times 10^5$ N/m²	 $P = 6.08 \times 10^5$ N/m²
Trans-2-butene/cis-2-butene	0.053	−0.0027	−0.014
Propylene/propane	−0.16	−0.071	−0.046
2-methyl pentane/*n*-hexane	−0.23	−0.099	−0.068
Ethylene/ethane	−0.23	−0.091	−0.076
Cis-2-butene/2-methyl pentane	−0.38	−0.15	−0.091
Ethane/trans-2-butene	−0.88	−0.30	−0.17

TABLE 2. FEED CONDITIONS AND PERFORMANCE SPECIFICATIONS (CASES 1 AND 2)

Feed conditions:	50% light component 50% heavy component fraction liquefied = 71% flow rate = 0.126 kg mole/s
Performance specifications:	light component mole fraction greater than 0.862 in distillate heavy component mole fraction greater than 0.862 in bottoms
Pressure:	set in a way that the reboiler and condenser are at subambient temperatures for the normal distillation and the condenser is approximately 305.6°K for the two-column distillation design
Number of stages:	100
Heat transfer area:	18.58 m² per pair of stages

In the first set of simulation runs, the evaluation was carried out for two mixtures: trans-2-butene/cis-2-butene and propylene/propane. Both systems are close boiling mixtures, the butenes being the closest boiling mixture that we have examined. The operating pressures were selected on the basis of the following considerations:

1. Both reboiler and condenser temperature should be subambient for conventional distillation.

2. The condenser temperature for SRV distillation should be above ambient, so that cooling water may be used instead of refrigeration.

3. The pressure difference in SRV distillation should be such that there is a temperature difference of approximately 27.8°K between the paired stages in the rectifying section and the stripping section.

A heat transfer area of 18.58 m² per pair of stages and an overall heat transfer coefficient of 567.8 J/m² · s · °K were assumed. The feed conditions and performance specifications are summarized in Table 2, and the results of simulation are given in Tables 3 and 4. In order to investigate the influence of the refrigerant on the outcome of this evaluation, the results in Table 4 were computed using two refrigerants of different characteristics: refrigerants 170 and 22 (Perry, 1973). However, the conclusions appear to be materially unaffected by the choice of the refrigerant.

For the butene mixture, the SRV distillation requires 15% less steam and 35% less cooling water in comparison with the conventional distillation. But for the propyl-

Table 3. Operating Conditions for Cases 1 and 2

	Conventional distillation		SRV distillation	
	Trans-2-butene/ cis-2-butene	Propylene/ propane	Trans-2-butene/ cis-2-butene	Propylene/ propane
Condenser temperature, °K	279.91	278.19	306.04	307.49
Reboiler temperature, °K	281.53	283.21	281.52	283.23
Valve temperature, °K	—	—	280.74	280.33
Rectifier pressure, N/m²	1.216×10^5	6.586×10^5	2.938×10^5	14.168×10^5
Stripper pressure, N/m²	1.216×10^5	6.586×10^5	1.216×10^5	6.586×10^5
Reboiler duty, W	30.023×10^6	8.209×10^6	19.484×10^6	3.219×10^6
Condenser duty, W	29.392×10^6	7.785×10^6	16.905×10^6	1.178×10^6
Compressor duty, W	—	—	2.864×10^6	1.321×10^6
Valve cooling, W	—	—	4.684×10^6	2.867×10^6
External reflux ratio	20	7.648	12.3	1.293

Table 4. Utility Requirements for Cases 1 and 2

	Conventional distillation		SRV distillation	
Mixture	Trans-2-butene/ cis-2-butene	Propylene/ propane	Trans-2-butene/ cis-2-butene	Propylene/ propane
(a) Refrigerant 22				
Cooling water, kg/s	860.57	235.24	558.42	91.98
Steam, kg/s	31.75	7.67	26.96	13.10
(b) Refrigerant 170				
Cooling water, kg/s	860.57	235.24	558.42	91.98
Steam, kg/s	46.92	11.46	28.90	14.27

Table 5. Feed Conditions and Performance Specifications (Case 3)

Feed conditions:	50% ethylene 50% ethane fraction liquefied = 71% feed rate = 0.126 kg mole/s
Performance specifications:	light component mole fraction greater than 0.99 in distillate heavy component mole fraction greater than 0.99 in bottoms
Pressure:	rectifier: 9.119×10^5, N/m² stripper: 3.040×10^5, N/m²
Number of stages:	30
Heat transfer area:	18.58 m² per pair of stages

Table 6. Operating Conditions for Case 3 (Ethylene/Ethane; Refrigerant 22)

	Conventional column	SRV column
Condenser temperature, °K	191.17	218.86
Reboiler temperature, °K	207.69	207.73
Valve temperature, °K	—	198.31
Rectifier pressure, N/m²	3.040×10^5	9.119×10^5
Stripper pressure, N/m²	3.040×10^5	3.040×10^5
Reboiler duty, W	2.482×10^6	1.495×10^6
Condenser duty, W	2.150×10^6	1.070×10^6
Compressor duty, W	—	0.509×10^6
Valve cooling, W	—	0.574×10^6
External reflux ratio	2.652	1.500

Table 7. Utility Requirements for Case 3 (Ethylene/Ethane)

	Conventional column	SRV column
(a) Refrigerant 22		
Steam, kg/s	19.42	8.46
Cooling water, kg/s	132.19	32.62
(b) Refrigerant 170		
Steam, kg/s	33.92	11.12
Cooling water, kg/s	184.84	42.27
(c) Propane and refrigerant 170		
Steam, kg/s	16.40	7.60
Cooling water, kg/s	130.05	29.47

ene/propane mixture, the steam consumption actually increases by 71% even though the cooling water decreases by 61% in going from the conventional distillation to the SRV distillation. The reversal is attributable to a much larger pressure difference between the rectifying section and the stripping section in the second case.

In the second set of simulation runs, the comparison was made at much lower operating temperatures. For this purpose the ethane/ethylene mixture was selected. Again, the operating pressures were selected according to the considerations given previously. The feed conditions and performance specifications are summarized in Table 5, and the results of simulation are given in Tables 6 and 7. In this case, the SRV distillation performed notably better than the conventional distillation. The steam consumption was reduced by 54% and the cooling water by 77%.

CONCLUSIONS

On the basis of our simulation studies it would appear that the SRV distillation offers some distinct advantages over the conventional distillation for the cryogenic separation of close boiling mixtures. The temperature range of operation appears to be the most significant factor in this comparison. The characteristics of the mixture and product specifications also play an important role. But the choice of the refrigerant does not seem to affect the outcome of this comparison materially.

In our investigation, a 54% reduction of steam consumption and a 77% reduction of cooling water were obtained for the most favorable case. This evaluation does not take any credit of the potential power recovery through the use of expanders, nor of the potential savings if "valve cooling" (cooling of reflux to the bubble point temperature) is not applied. Furthermore, less compression work will be required if a smaller temperature difference (< 27.8°K) between the paired stages in the rectifying and the stripping sections is allowed.

Further investigation is underway to delineate the region of favorable operation for the SRV distillation of multicomponent mixtures and the physical implementation of SRV distillation schemes.

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NOTATION

A = area, m^2
b = bottoms flow rate, kg-mole/s
d = distillate flow rate, kg-mole/s
F_j = flow rate of feed to stage j, kg-mole/s
F_{ij} = flow rate of component i in the feed to stage j, kg-mole/s
H_j = enthalpy of the vapor on stage j, J/kg-mole
H_j^* = enthalpy of the vapor entering the rectifying section after compression, J/kg-mole
h_j = enthalpy of the liquid on stage j, J/kg-mole
h_j^* = enthalpy of the liquid entering the stripping section after expansion, J/kg-mole
h_{Fj} = enthalpy of the feed stream into stage j, J/kg-mole
I = number of components
K_{ij} = vaporization equilibrium ratio for component i on stage j
L_j = liquid flow rate out of stage j, kg-mole/s
n = number of stages; stages 1 and n denote the condenser and reboiler, respectively
P = pressure, N/m^2
Q_j = heat removal rate from stage j, J/s
T = temperature, °K
U_j = liquid sidestream withdraw rate from stage j, kg-mole/s
U_{ov} = overall heat transfer coefficient, J/m^2 · s · °K
V_j = vapor flow rate out of stage j, kg-mole/s
W_j = vapor sidestream withdraw rate from stage j, kg-mole/s
x_{ij} = liquid mole fraction of component i on stage j
y_{ij} = vapor mole fraction of component i on stage j
α = relative volatility

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System Structures for Process Simulation

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The plex data structure is proposed for use in an advanced computing system to model chemical processes. The plex is shown to permit increased modularity and flexibility over systems with dimensioned array structures. Two methods are suggested to create and operate upon the plex: the problem oriented language and the problem oriented calling programs. The concept of a routing plex is introduced as a means for specifying the path of calculations when building block routines call upon other routines and choices exist at each level.

SCOPE

This paper presents concepts for design of an advanced computing system to meet the needs of process engineering in the 1980's. The requirements for such a system were discussed earlier (Evans and Seider, 1976). In this paper, we consider trends in process engineering and digital computation and their impact on system design. Two aspects to design of the system are examined: data structure and programs.