Separation Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

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To cite this Article Peridis, Stavros , Magoulas, Kostis and Tassios, Dimitrios(1993) 'Sensitivity of Distillation Column Design to Uncertainties in Vapor-Liquid Equilibrium Information', Separation Science and Technology, 28: 9, 1753 — 1767

To link to this Article: DOI: 10.1080/01496399308019040

URL: http://dx.doi.org/10.1080/01496399308019040

SEPARATION SCIENCE AND TECHNOLOGY, **28**(9), pp. 1753–1767, 1993

Sensitivity of Distillation Column Design to Uncertainties in Vapor–Liquid Equilibrium Information

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ABSTRACT

The sensitivity of distillation column design [number of stages (N) and reflux ratio (R)] to changes in the mean relative volatility (α) across the column is examined to demonstrate the effect that uncertainties in the required vapor–liquid equilibrium (VLE) information has on N and R. The results, presented in graphic form for different levels of α, provide the design engineer with a simple method of establishing the required degree of accuracy in the VLE information used for a given separation. The sensitivity increases, as expected, with decreasing values of α, becoming very pronounced for difficult separations, but it is significant even for easier ones. Thus, for $\alpha = 1.1$, a 2% reduction in α leads to a 80% increase in N or an over 120% increase in R, while for $\alpha = 1.5$ the corresponding increases are about 20 and 25%, respectively. The dependence of this sensitivity on design parameters, such as the ratio of the key components in the feed, feed thermal condition, etc., is also examined. The effect of the sources of uncertainty in the VLE information: the values of the interaction coefficient and, on occasion, of the critical properties and acentric factor, is then demonstrated with two examples.

INTRODUCTION

Design of distillation columns is often based on inexact thermodynamic data and/or correlations. The effect of this uncertainty on the number of stages (N) and the reflux ratio (R), required for a given separation, has been presented through some specific systems by Nelson et al. (1) and Hernandez et al. (2), while Macchietto et al. (3) examined its effect on the purity of the products obtained for the CH_4–C_2H_4–C_2H_6–C_3H_6 system and a given N and R.

A systematic study of the sensitivity of N and R to uncertainties in the vapor–liquid equilibrium (VLE) information is presented here. To this purpose, the sensitivity of N and R is demonstrated as a function of the changes in the mean relative volatility (α) of the key components of the mixture for a wide range of α values:

$$\alpha = [\alpha_1 \, \alpha_2 \, \alpha_3 \, . \, . \, . \, \alpha_i \, . \, . \, . \, \alpha_N]^{1/N} \tag{1}$$

where 1, 2, . . . , i, . . . , N are the 1st, 2nd, . . . , ith, . . . , and Nth stage, and

$$\alpha_i = \frac{(y_i/x_i)_{\mathrm{LK}}}{(y_i/x_i)_{\mathrm{HK}}} \tag{2}$$

where the subscripts LK and HK refer to the light and heavy keys, respectively.

Six values of α (1.10, 1.15, 1.20, 1.25, 1.50, and 1.80), referred to as "base" values, were selected as covering the range from very difficult to easy separations, using binary nonpolar systems modeled with the Graboski and Daubert (4) version of the Soave–Redlich–Kwong (SRK-GD) equation of state (EoS). Design factors that could affect this sensitivity:

a. Presence of nonkey components
b. Thermal quality of the feed
c. Ratio R/R_{min}, where R_{min} is the minimum reflux ratio
d. Ratio of light to heavy key in the feed
e. Product purity

are then examined.

Finally, the effect of the two main sources of uncertainties in the thermodynamic modeling of such systems through an EoS [values of the interaction coefficients (k_{ij}) and, on occasion, of the critical properties and acentric factor (T_c, P_c, ω)] are considered by using two examples.

PROCEDURE

To attain the selected base levels of relative volatility, the binary systems presented in Table 1 were used. Product specifications were set to 0.01 mol fraction of the light and heavy keys in the bottoms and distillate, respectively, and a saturated liquid feed containing a mole ratio of light to heavy keys equal to 65/35 was used.

Tray-to-tray calculations were carried out using the Naphtali–Sandholm (5) rigorous model, as modified by Christiansen et al. (6). The Fenske–Underwood–Gilliland (Yang, 7) short-cut model was employed to estimate the minimum reflux ratio (R_{min}) and the number of trays using R/R_{min} =

TABLE 1
Mixtures and Operating Conditions for the Selected "Base" Levels of Relative Volatility and the Corresponding N and R Values[a]

α	Mixture	P (atm)	N	R	T_{top} (°C)
1.10	$C_3^=-C_3$	25.0	166	20.0	59.7
1.15	$C_3^=-C_3$	12.5	117	13.0	28.5
1.20	iC_5-nC_5	4.4	93	9.7	78.8
1.25	iC_5-nC_5	2.1	75	7.7	51.4
1.50	$C_6H_{14}{}^b-nC_6H_{14}$	3.8	43	3.9	98.8
1.80	C_3-iC_4	16.1	30	2.4	48.1

[a] $R/R_{min} = 1.3$. Feed: Saturated liquid with $x_{LK}/x_{HK} = 65/35$. Purity: 0.01 mol fraction of the LK and HK in the bottoms and distillate, respectively.

[b] 2,2-Dimethyl butane.

1.3. The feed tray location was estimated from the Kirkbride equation (8). These were used as input data in the rigorous model. The operating pressure of the column was then determined to achieve the desired base value of the mean relative volatility, along with the number of stages and optimum feed tray location required to meet the product specifications. A value of $k_{ij} = 0.0$, referred to as the base value, was used, and a negligible pressure drop across the column was assumed. The N and R values obtained, also referred to as base values, operating pressures (P), and the corresponding top temperatures (T_{top}) for the selected base α values are presented in Table 1.

Changes in the relative volatility, leading to a reduction of the base value, were generated by increasing the interaction coefficient k_{ij} from its base zero value. To determine the sensitivity of N to α, N and the feed tray location were varied by trial and error until the product specifications were met, keeping the reflux ratio constant and equal to its base value. The same procedure was used to study the sensitivity of the reflux ratio to α, but now the number of stages was kept constant and equal to its base value. The feed tray location was also set equal to its base value because it was found to have an insignificant effect on R.

RESULTS AND DISCUSSION

Figures 1 and 2 demonstrate the sensitivity of the number of stages and reflux ratio, respectively, to reductions in the relative volatility using the systems and conditions of Table 1. The trend in the two figures is the same, but the reflux ratio is more sensitive than the number of stages. Thus, the same percent reduction in the relative volatility leads to a larger

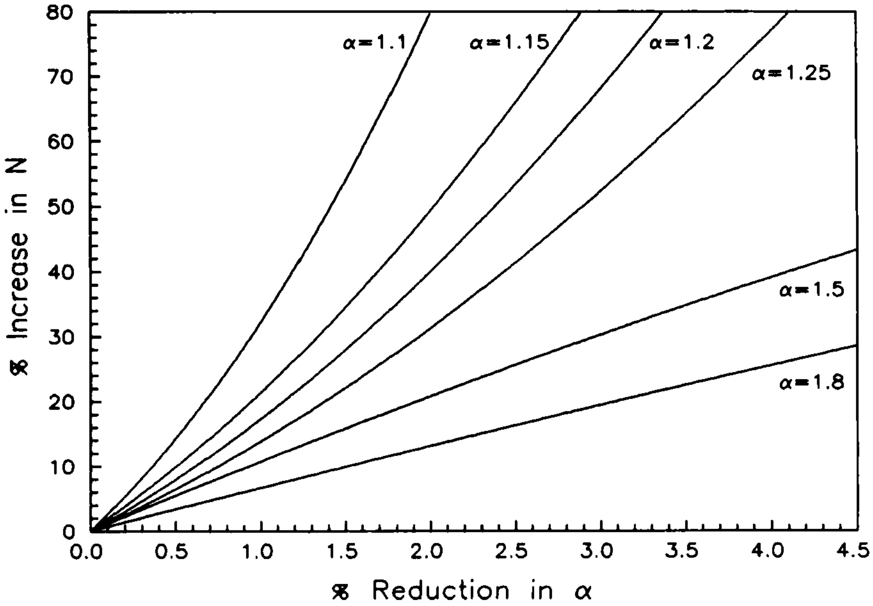

FIG. 1 Sensitivity of the number of stages to the relative volatility while holding the reflux ratio equal to its base value.

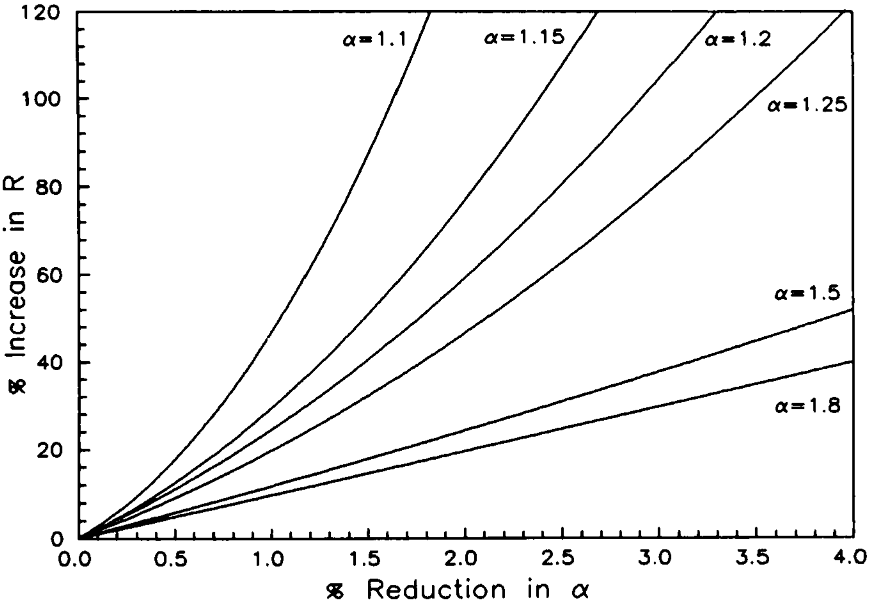

FIG. 2 Sensitivity of the reflux ratio to the relative volatility while holding the number of stages equal to its base value.

change in the reflux ratio than in the number of stages. Notice that, as shown in Figs. 3 and 4, these changes represent dramatic increases in N and R for difficult separations, but also significant ones for easier separations. Thus, for $\alpha = 1.1$, a 2.0% reduction in the mean relative volatility yields an 80% increase in the number of stages, which corresponds to about 130 stages; or an over 120% increase in the reflux ratio, which corresponds to an over 24 units increase in its value. On the other hand, for $\alpha = 1.5$, the same reduction in the relative volatility yields a 21% increase in the number of stages, which corresponds to 9 stages; or a 24% increase in reflux ratio, which corresponds to a 0.9 unit increase in its value.

Figures 1 through 4 were developed using the binary systems, $R/R_{\min}$, feed composition, thermal condition, and product specifications presented in Table 1. We examine next the effect of these parameters on the sensitivity of N and R to uncertainties in the α value.

The effect of the presence of nonkey components on the sensitivity of N and R to α (Figs. 1 and 2) is, as expected, not significant (not shown). The same applies to feed thermal condition and product purity, provided that the latter is close to the levels used in this study.

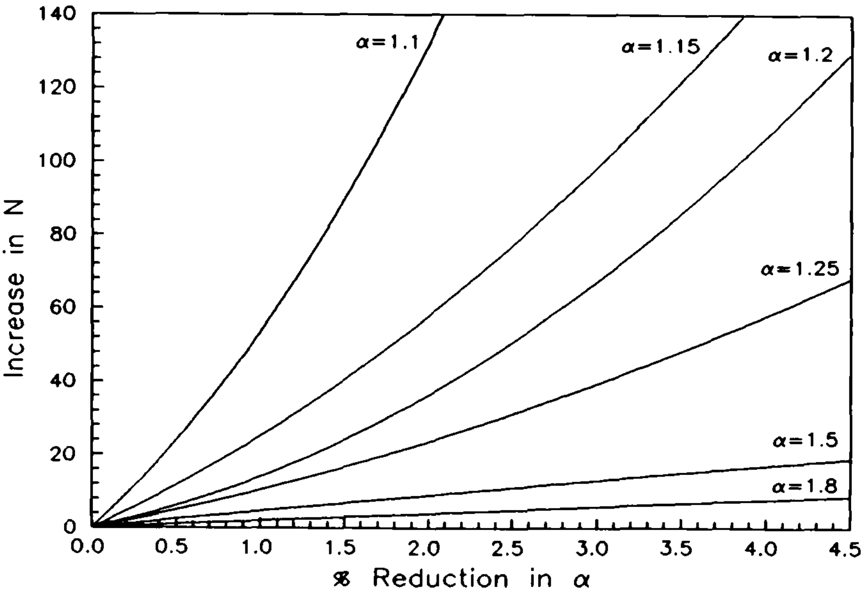

FIG. 3 Increase of the number of stages with decreasing values of the relative volatility while holding the reflux ratio equal to its base value.

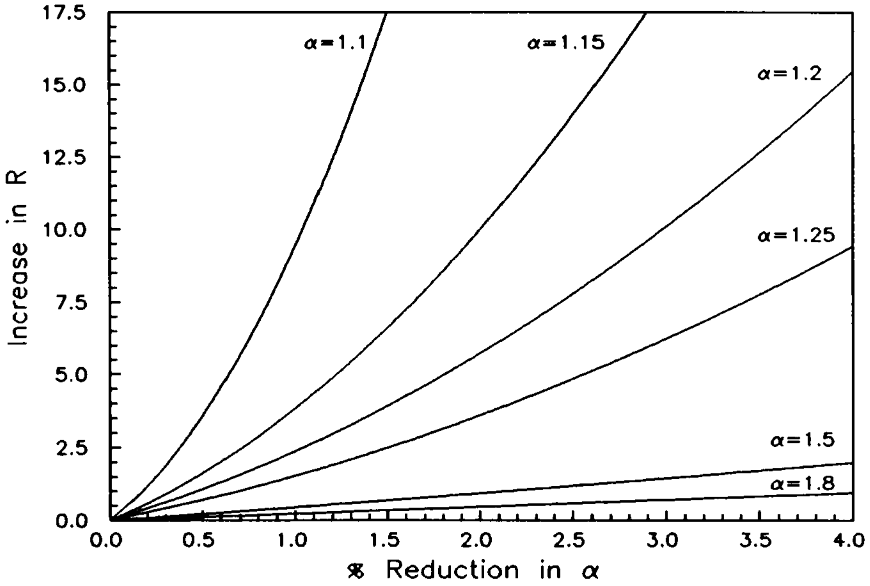

FIG. 4 Increase of the reflux ratio with decreasing values of the relative volatility while holding the number of stages equal to its base value.

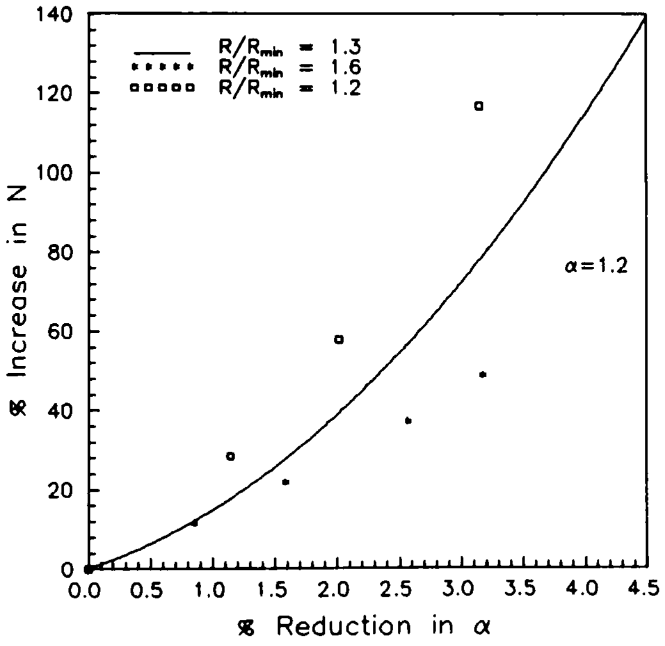

FIG. 5 The effect of the ratio $R/R_{\min}$ on the sensitivity of N to α.

On the other hand, the value of R/R_{min} has a significant effect on the sensitivity of N and R to α, as Figs. 5 and 6 demonstrate for $\alpha = 1.2$. Thus, for a 3% reduction in α and $R/R_{\text{min}} = 1.2$, 1.3, and 1.6, the corresponding increases in N are 108, 72, and 45%, respectively, while the opposite trend is observed for R: 76, 104, and over 120%, respectively. This reverse trend is due to the fact that as R/R_{min} decreases, the base value of N increases; for example, from 93 at $R/R_{\text{min}} = 1.3$ to 102 at $R/R_{\text{min}} = 1.2$, both for $\alpha = 1.2$.

Finally, the ratio of the key components in the feed has a pronounced effect on the sensitivity of N to α, but a less important one on that of R, as Figs. 7 and 8 respectively demonstrate for $\alpha = 1.25$. The drastic reduction in the sensitivity of N to α, as the (LK/HK) ratio in the feed changes from 65/35 to 35/65, results from the fact that, due to the inversion of the material balance, the minimum reflux ratio increases drastically, by 90% in this case.

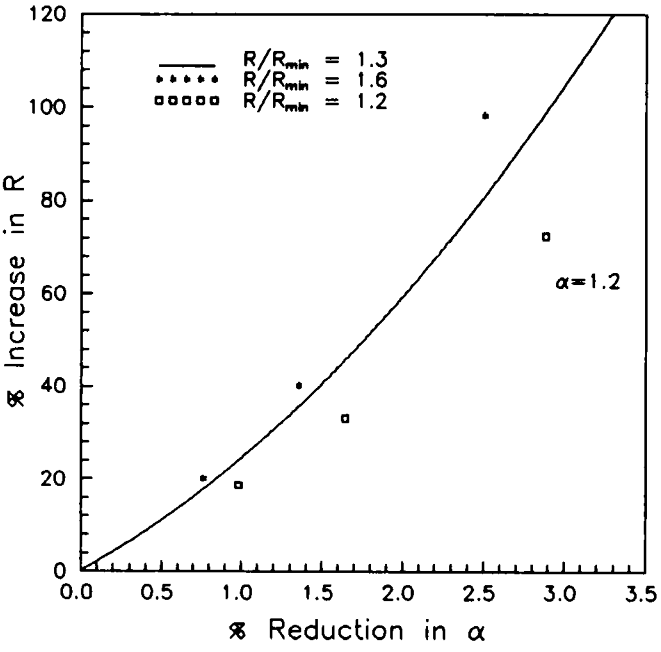

FIG. 6 The effect of the ratio R/R_{min} on the sensitivity of R to α.

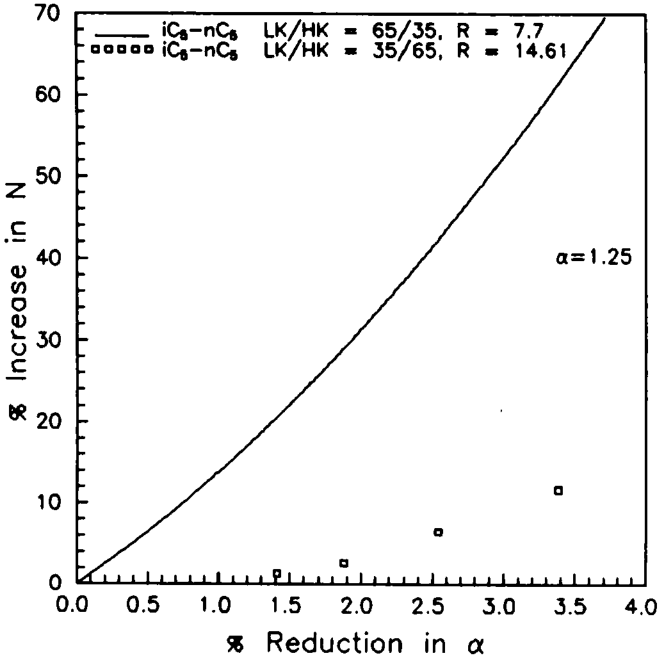

FIG. 7 Effect of the ratio of the key components in the feed on the sensitivity of N to α.

SOURCES OF UNCERTAINTY IN EVALUATING THE RELATIVE VOLATILITY AND THEIR EFFECT ON *N* AND *R*

For nonpolar/slightly polar systems the main source of uncertainty in the VLE information, and consequently in the mean relative volatility, is the value of the interaction coefficient k_{ij}; and, on occasion, the values of the critical properties T_c, P_c, and the acentric factor ω. The effect of these uncertainties on the number of stages and reflux ratio is demonstrated next with the propylene–propane and the ethyl benzene–styrene separations. Product purity of 99% (mol), $R/R_{\text{min}} = 1.3$, and saturated liquid feed with $x_{\text{LK}}/x_{\text{HK}} = 65/35$ are specified again. The propylene–propane system has been studied in detail by Hernandez et al. (2) for the sensitivity of design on the EoS used for the thermodynamic modeling (BWR, SRK, and PR).

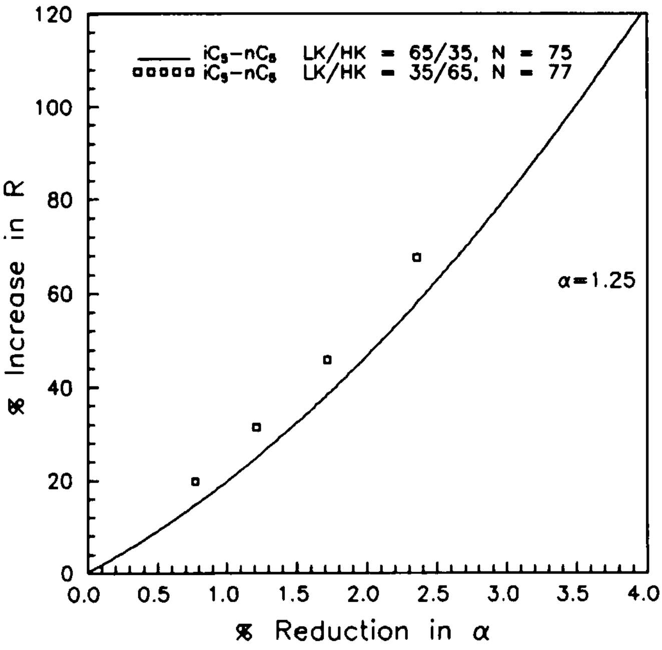

FIG. 8 Effect of the ratio of the key components in the feed on the sensitivity of R to α.

Propylene–Propane Separation

The recommended operating pressure for this separation is 120 psia, about 8 bar (Kenney, 9). There is no uncertainty in the T_c, P_c, and ω values of the two components, but for k_{ij} Knapp et al. (10) report—based on data sets from different sources—five values, which are presented in Table 2. These data sets cover, or are close to, the range of operating

TABLE 2
Interaction Coefficient Values (k_{ij}) for the System Propylene–Propane (Knapp et al.)

T_{min} (K)	T_{max} (K)	P_{min} (bar)	P_{max} (bar)	k_{ij}
223	239	0.72	1.83	0.014
269	333	4.39	23.5	0.001
260	360	3.42	41.6	0.004
310	344	13.00	31.3	0.000
223	360	0.72	41.6	0.003

conditions for the distillation column, except for the first, which is included to indicate the extent of variation in the k_{ij} value.

Using as base value $k_{ij} = 0.0$, the typical choice for hydrocarbon systems of similar size, and $R/R_{\min} = 1.3$: $\alpha = 1.175$, $N = 103$, and $R = 11.07$ are obtained.

The effect of the uncertainty in the k_{ij} values on the mean relative volatility is shown graphically in Fig. 9 for $N = 103$, and it is significant in spite of the very small variation in the k_{ij} value. The same is observed when $R = 11.07$ is used. Consequently, as Figs. 1 through 4 suggest, the effect on the number of stages and reflux ratio should be also significant. This is indeed the case, as Fig. 10 demonstrates: significant variations in N and in R are observed, especially if the value of 0.0075, recommended by Hernandez et al. (2) and based on the experimental data of Manley and Swift (11), is considered.

Ethyl Benzene–Styrene Separation

This separation involves top of the column pressures below 100 mmHg to avoid high pressures—and thus high temperatures—at the bottom of

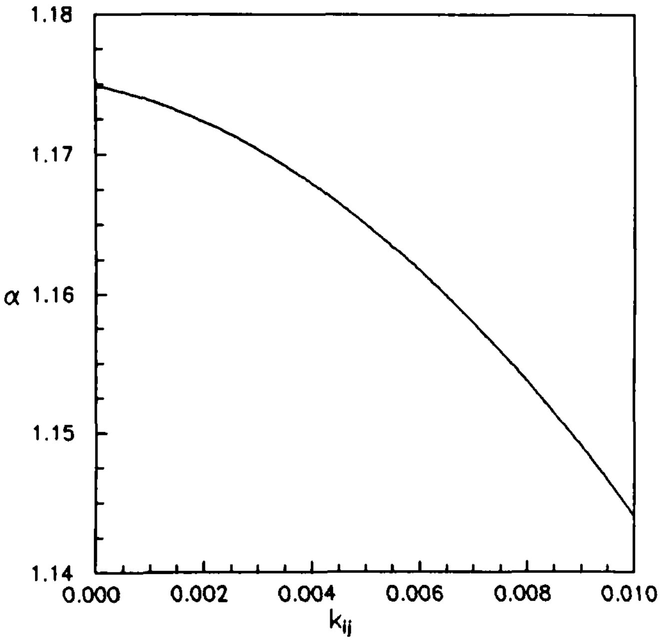

FIG. 9 The effect of the uncertainty in k_{ij} on α for N equal to its base value of 103 (k_{ij} = 0.0) for the system propylene–propane.

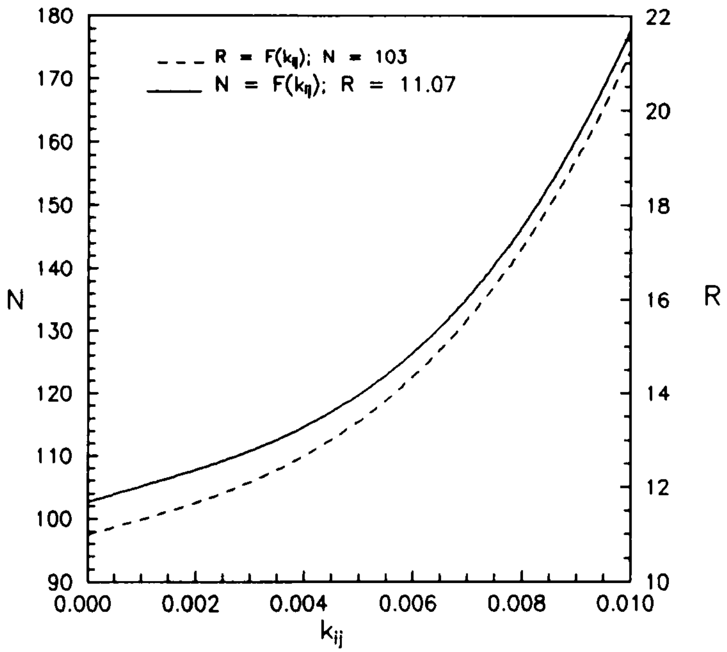

FIG. 10 The effect of the uncertainty in k_{ij} on N and R for the system propylene–propane.

the column that could lead to styrene polymerization. A pressure of 100 mmHg was used here since no pressure drop across the column is accounted for. Two sets of VLE data by the late Professor Van Winkle and his coworkers, as presented by Hirata et al. (12), are available at this pressure.

The available values for T_c, P_c, and ω from the two main sources for such properties: Reid, Prausnitz, and Poling (RPP, 13) and Daubert and Danner (DD, 14) are presented in Table 3. The values are very close but, as Table 4 indicates, lead to significantly different k_{ij} values when

TABLE 3
Critical Properties and Acentric Factors for the System Ethyl Benzene–Styrene

Source	Compound	T_c (K)	P_c (bar)	ω
RPP	Ethyl benzene	617.20	36.00	0.3020
DD	Ethyl benzene	617.17	36.09	0.3036
RPP	Styrene	647.00	39.90	0.2570
DD	Styrene	648.00	40.00	0.2356

TABLE 4
Interaction Coefficients and Quality of Description of the VLE Data of Table 3[a]

				Average absolute % error in	
T_c, P_c, ω	VLE	n	k_{ij}	P	α
RPP	A	9	0.013	1.178	5.373
RPP	B	12	0.005	1.556	5.074
DD	A	9	−0.001	2.120	16.18
DD	B	12	−0.008	3.507	10.08

[a] n = number of experimental data points. A = White and Van Winkle, 1954. B = Chaiyavech and Van Winkle, 1959.

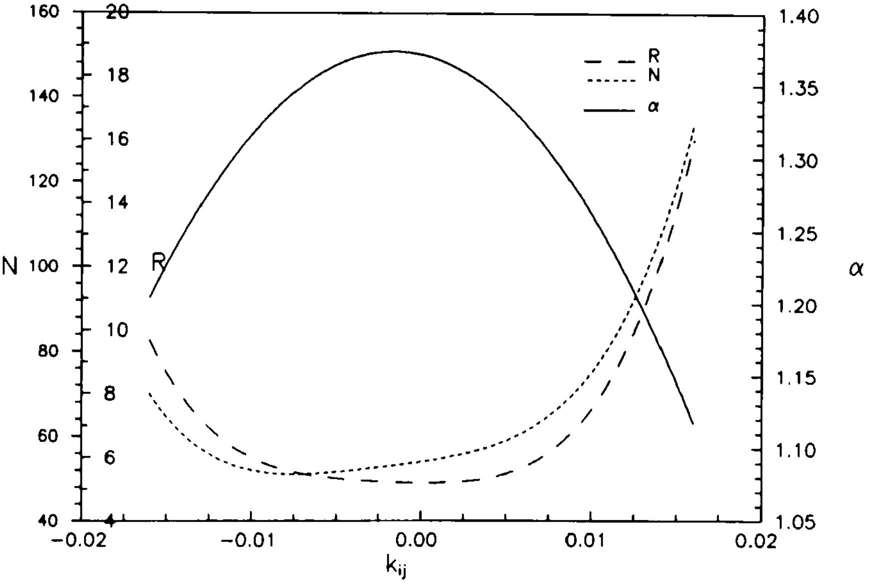

FIG. 11 The effect of the uncertainty in the k_{ij} value on α, N, and R for the ethyl benzene–styrene system. T_c, P_c, and ω values from RPP.

correlating the two sets of VLE data. [The k_{ij} values were obtained using the SRK-GD EoS and minimizing the relative error (Q) between experimental (exp) and calculated (calc) total pressures:

$$Q = \sum\left[\frac{P^{\text{calc}} - P^{\text{exp}}}{P^{\text{exp}}}\right]_i^2 \tag{3}$$

where the summation covers all data points. The corresponding values for the average absolute percent deviation in P and α are also included in Table 4.]

Figures 11 and 12 present the variation of the mean relative volatility across the column with k_{ij} for the two sets of T_c, P_c, and ω values. Notice the pronounced effect that the small differences in the two sets of T_c, P_c, and ω values have on the variation of α, and consequently on N and R, with k_{ij}: for $k_{ij} = 0.0$, for example, the RPP values give $R = 5.2$ and $N = 54$; the DD ones give $R = 8.0$ and $N = 77$, which represent differences of over 50 and 40%, respectively.

The effect of the VLE data is still more pronounced: use, for example, of the T_c, P_c, and ω set that provides the best description of the VLE

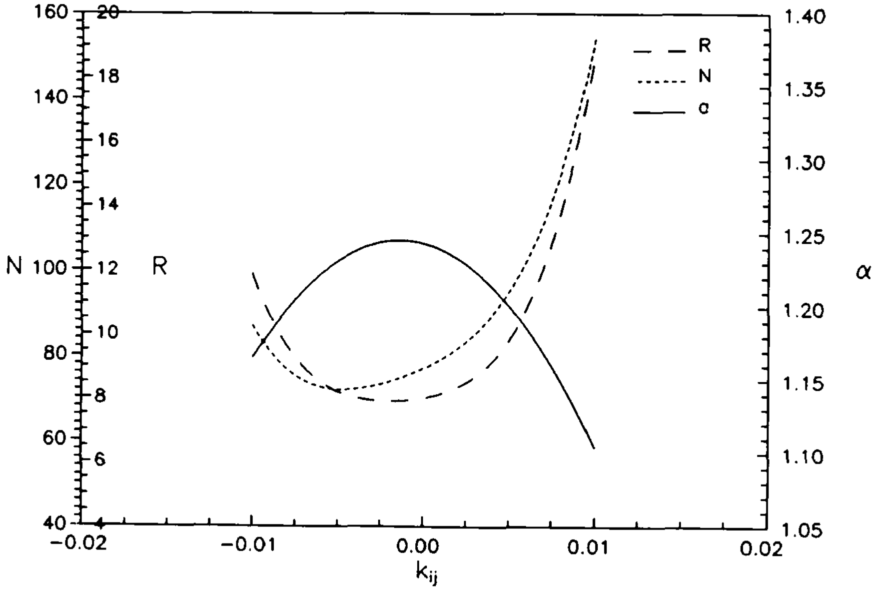

FIG. 12 The effect of the uncertainty in the k_{ij} value on α, N, and R for the ethyl benzene–styrene system. T_c, P_c, and ω values from DD.

data (RPP), and the corresponding k_{ij} values, leads to N and R values respectively of 97 and 10.5 (A) and 59 and 5.5 (B), differences of over 60 and 90%.

It should be mentioned that in this case both R and N are varied to meet the product specifications, holding $R/R_{\min} = 1.3$ and determining $R_{\min}$ at each α value. Finally, the fact that for the same α and R, two N values are obtained—one for $k_{ij} > 0.0$ and one for $k_{ij} < 0.0$—should not be surprising. The same mean value of α does not mean that the variation of the relative volatility in the column is exactly the same, a fact that affects N but not R.

CONCLUSIONS

The sensitivity of the number of trays and reflux ratio for a given separation to the vapor–liquid equilibrium information used is established at different levels of the mean relative volatility (α). The results, presented in graphics form at different levels of α, provide the design engineer with a simple method of establishing the required degree of accuracy in the VLE information used for a given separation. Thus, for a moderately difficult separation ($\alpha = 1.2$), a reduction of only 3% in α leads to about 67 and 105% increases in N and R, respectively, for $R/R_{\min} = 1.3$, indicating that the accuracy of the VLE information should be carefully evaluated before they are used for column design. The errors are much reduced for easier separations; for example, for $\alpha = 1.5$, the same change in α leads to errors of 30 and 36%, respectively, less than half of the aforementioned values but still not ignorable. Factors that significantly affect this sensitivity are the ratio of the key components in the feed and the $R/R_{\min}$ ratio, but not the presence of nonkey components, the thermal condition of the feed, and the purity of the products.

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Received by editor July 22, 1992