Table 5

Stream composition, Example 3

Number	Component	Feed, %	Relative volatility α_i
1	Isoprene	16.00	2.857
2	3-methylpentene-1 (LK)	30.00	1.297
3	2-methylpentene-1 (HK)	24.00	1.000
4	2,3-dimethylbutane-2	30.00	0.728

Underwood's method

If an infinite, or nearly infinite, number of equilibrium stages is involved, a zone of constant composition must exist in the fractionating column. In this instance, there is no measurable change in composition of liquid or vapor from stage to stage.

Under these conditions, the reflux ratio can be defined as the minimum reflux ratio, R_{min}, with respect to a given separation of two-key components (light key and heavy key).[11] Equation 21 shows R_{min} for component i in the distillate. Underwood's constant, θ, or the root of the equation, must lie between the relative volatilities of the light and heavy keys (α_{HK} and α_{LK}). The number of components is n.

Equation 22 shows the relationship for the feed, where q is the fraction of feed that is liquid at the feed tray temperature and pressure. For a bubble-point feed, q = 1.0, for a dew-point feed, q = 0.

The minimum reflux ratio is determined from Equation 22 by substituting into Equation 21.

Describing Gilliland's graph

Many equations have been proposed to describe Gilliland's curve for multicomponent distillation. However, the difficulty with some of these equations has been in meeting the end conditions of X = 0, Y = 1 and X = 1, Y = 0. A review of the many equations proposed by these authors is shown in Equations 23-34.

From the equations listed, McCormick's gives a good agreement in the normal operating range of real towers. It is, thus, employed in the program.

The reflux ratio, R, is calculated as a multiple of the minimum reflux ratio, R_{min} (Equation 35). The multiplier FACTOR generally varies from 1.2 to about 1.5 for conventional columns, but because of economic situations, the range is now between 1.05 to 1.20.

Kirkbride's feed-plate location

After the minimum number of stages and the minimum reflux ratio have been determined, the number of theoretical stages is then calculated. The ratio of the number of plates above the feed stage (including the partial condenser) to the number below the feed stage (including the reboiler) can be obtained using Kirkbride's empirical equation.[20]

The equation was developed on the basis that the ratio of rectifying trays to stripping trays is a function of:

- The fraction of the heavy-key component (in the feed) removed in the overhead
- The fraction of the light-key component removed in the bottoms
- The concentration of the heavy-key component in the overhead
- The concentration of the light-key component in the bottoms.

Equation 36 shows the relationship.

Examples

Three examples are used to show the operation of the program.

Example 1. The feed to a butane-pentane splitter of the composition shown in Table 1 is to be fractionated into a distillate product containing 95% of the n-butane contained in the feed, and a bottoms product containing 95% of the iso-pentane in the feed. The reflux ratio for the fractionation will be 1.3 R_{min} and the column pressure 100 psia at the top plate. The reflux and feed are at their bubble-point temperatures. The feed composition and equilibrium constants are shown in Table 1.

The short-cut method is used to determine the recoveries of the components in the distillate and bottoms products, the minimum number of stages, the minimum reflux ratio, the actual number of theoretical plates, and the location of the feed plate. The results of the program execution are shown in Table 2.

Example 2. Propane (LK) and butadiene (HK) are separated in the presence of propylene, butane, and pentane. The desired recovery of both keys is 99% at 400 psia.

The feed is liquid at its bubble-point temperature. If the reflux ratio for the column is 1.37 R_{min}, calculate the feed distribution between the column distillate and bottoms, the minimum number of stages, the minimum reflux ratio, the actual number of stages, and the location of the feed plate.

Stream compositions are shown in Table 3, and the results are shown in Table 4.

Example 3. Determine the minimum reflux ratio, minimum number of plates, equilibrium number of plates, and the location of the feed plate for the separation of 3-methylpentene-1, and 2-methylpentene-1 in the presence of isoprene and 2,3-dimethylbutene-2.

Desired recovery of both

Table 6

Example 3 results

INPUT

Input number of components?	4
Do you want equilibrium constants, Yes/No?	N
Input feed and relative volatility of each component	16.0 2.857
	30.0 1.297
	24.0 1.000
	30.0 0.728
Input recoveries of light and heavy keys?	0.99 0.99
Input position of the heavy key component?	3
Input thermal feed condition Q?	1.0
Input factor for the reflux ratio?	1.15

OUTPUT

Multicomponent system fractionation

Component number	Feed moles	Rel. volatility alpha	Distillate %	Distillate Moles	Bottom, %	Bottom Moles
1	16.0000	2.8570	100.0000	16.0000	0.0000	0.0000
2	30.0000	1.2970	99.0000	29.7000	1.0000	0.3000
3	24.0000	1.0000	1.0000	0.2400	99.0000	23.7600
4	30.0000	0.7280	0.0000	0.0000	100.0000	30.0000

The heavy key component number is:	3
Percentage recovery of the light key component in the distillate is:	99.00 %
Percentage recovery of the bottom key component in the bottoms is:	99.00 %
Minimum number of stages is:	35.3
Total moles in the distillate is:	45.9400
Total moles in the bottoms is:	54.0600
Underwood constant:	1.1231
Minimum reflux ratio:	4.3544
Actual reflux ratio:	5.0075
Number of theoretical plates in the column:	76.1
The position of the feed plate is:	38.3
Do you want to print the results of the program? Yes/No	