Table 1

Ways to produce two-phase mixture

Initial	Action to produce two-phase mixture
Gas	Cool, possibly after initial compression
Gas	Expand through a valve or an engine
Liquid	Heat to achieve partial vaporization
Liquid	Reduce pressure through a valve, if close to saturation

Table 2

Equilibrium flash criteria

	$f_1 = \sum_{i=1}^{n} K_i n_i$	$f_2 = \sum_{i=1}^{n} n_i K_i$
Subcooled liquid	<1	>1
Bubble point	=1	>1
Two-phase condition	>1	>1
Dew point	>1	=1
Superheated vapor	>1	<1

where: T_{bp} is the bubble point temperature, T_s is the specified temperature, and T_{dp} is the dew point temperature.

The existence of a valid two-phase flash can be verified with the design equations for the bubble point, dew point, and equilibrium data calculated at the specified pressure and temperature.

The design equations for the bubble and dew points are:

Bubble point:

$$f_1 = \sum_{i=1}^{n} K_i X_i \quad (1)$$

Dew point:

$$f_2 = \sum_{i=1}^{n} Y_i / K_i \quad (2)$$

Table 2 illustrates the phase condition using the liquid-vapor data associated with the specified pressure and temperature.

From Table 2, the condition for a valid two-phase equilibrium flash is (see box for nomenclature):

$$f_1 = \sum_{i=1}^{n} K_i n_i > 1.0 \quad (3)$$

$$f_2 = \sum_{i=1}^{n} n_i / K_i > 1.0 \quad (4)$$

Feed analyses in terms of component concentrations are normally not available for complex hydrocarbon mixtures with a final boiling point more than about 38° C. (e.g., n-pentane) unless such a feed is broken down into pseudo components (narrow boiling fractions). This enables the mole fraction and equilibrium constant, K, to be estimated and, consequently, flash calculation of the mixture can be carried out.[5] A continuous equilibrium flash fractionation process is shown in Fig. 1.

Efficient techniques for the solution of the trial-and-error calculations necessary in multicomponent flash computations are given by Smith, Hengstebeck, King, and Oliver.[6-9] However, the iterative convergence method first suggested by Oliver, and later modifed by Kostecke, is employed in the program.[1,2]

Table 3

Nine-component mixture (Example 1)

Field stream data

Component Number	Component Name	Feed, moles/r	Equilibrium constant, K
1	CH_4	2,752	7.2
2	C_2H_6	1,634	1.65
3	C_3H_8	2,918	0.54
4	iC_4H_{10}	537	0.25
5	nC_4H_{10}	1,718	0.185
6	iC_5H_{12}	172	0.088
7	nC_5H_{12}	218	0.069
8	C_6H_{14}	47	0.028
9	C_7H_{16}	4	0.00078

Input

Input flash temperature, °F.? 90
Input flash pressure, psia? 370
Input number of components? 9
Input feed and equilibrium K of each component? 2,752.0 7.2
1,634.0 1.65
2,918.0 0.54
537.0 0.25
1,718.0 0.185
172.0 0.088
218.0 0.069
47.0 0.028
4.0 0.00078

Output

Multicomponent equilibrium flash calculation at 90.0° F. and 370.0 psi

Component number	K-value	Feed Moles/hr	Feed Mole frac.	Liquid Moles/hr	Liquid Mole frac.	Vapor Moles/hr	Vapor Mole frac.
1	7.200	2,752.000	0.275	388.353	0.072	2,363.647	0.516
2	1.650	1,634.000	0.163	682.316	0.126	951.684	0.208
3	0.540	2,918.000	0.292	2,003.467	0.370	914.533	0.200
4	0.250	537.000	0.054	443.314	0.082	93.686	0.020
5	0.185	1,718.000	0.172	1,485.664	0.274	232.336	0.051
6	0.088	172.000	0.017	160.091	0.030	11.909	0.003
7	0.069	218.000	0.022	205.985	0.038	12.015	0.003
8	0.028	47.000	0.005	45.913	0.008	1.087	0.000
9	0.001	4.000	0.000	3.997	0.001	0.003	0.000
Totals		**10,000.000**	**1.000**	**5,419.100**	**1.000**	**4,580.897**	**1.000**

Do you want to terminate the program? Yes/No

Flash calculation equations

The equations used in the program for multicomponent equilibrium flash calculations are:

$$f_1 = \sum_{i=1}^{n} n_i K_i < 1 \text{ all liquid} \quad (5)$$

$$f_2 = \sum_{i=1}^{n} n_i / K_i < 1 \text{ all vapor} \quad (6)$$

$$C_i = [M_i(K_i - 1)(R+1)]/(K_i + R) \quad (7)$$

where: R = the liquid-vapor (L/V) ratio.

The new L/V ratio for each iterative calculation, R′, is determined from:

$$R' = [FR - E(R+1)]/[F + E(R+1)] \quad (8)$$

where the constants E and F are determined from:

$$E = \sum_{i=1}^{n} C_i \quad (9)$$

$$F = \sum_{i=1}^{n} (C_i)^2 / M_i \quad (10)$$

The computation then de-