Equilibrium flash calculations quickly computed on PC

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Equilibrium flash calculations can be computed quickly by an interactive Fortran program developed for personal computers. The program determines the equilibrium separation of a stream for multicomponent mixtures in oil, gas, and chemical processes, resulting in a liquid-vapor equilibrium mixture.

Results are obtained much faster than with previously published programs.[1-4]

Flash vaporization calculations involving multicomponent mixtures are essential to the design and successful operation of many processes. These calculations are often required to determine the condition of the feed to a fractionation column or to determine the flow of vapor from a reboiler or condenser.

Flash calculations often involve trial-and-error solutions which are time consuming, tedious, and subject to error if performed manually. Previous calculation procedures involved the use of programmable calculators which, with the growing use of personal computers, are becoming obsolete.

Multicomponent flash (isothermal and adiabatic) computations are incorporated as part of overall process simulation and equipment design. However, single-stage flash fractionation processes are also employed to obtain a separation of the light components in a feed and as a preliminary step before a multicomponent fractionation column, such as crude distillation.

Table 1 lists ways of producing two-phase mixtures from a single phase at appropriate conditions. The last process in the table typifies the well-head separation that takes place in an oil field. It is termed a flash process because vapor forms as a result of rapidly dropping the pressure.

Fundamentals

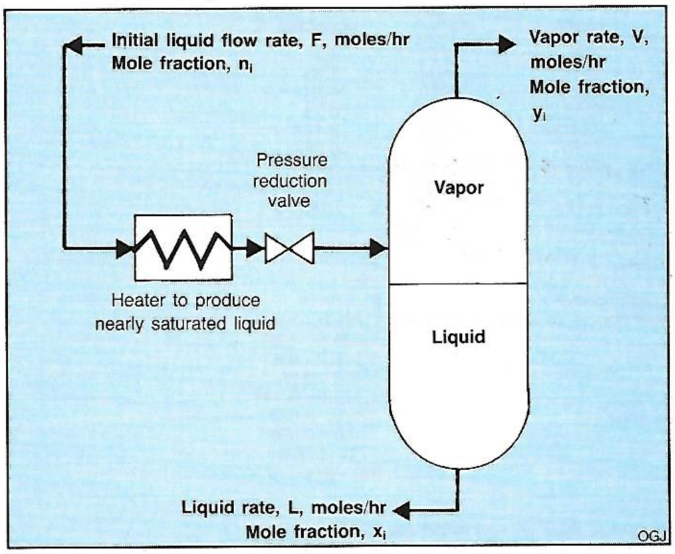
To carry out an appropriate flash calculation, the pressure, P, and the temperature, T, must be known. If the values of P and T in the separating vessel are fixed, the value of P must not be so high that two phases cannot exist at any value of T.

Nor must T lie outside of the bubble point and dew point range corresponding to P. For a valid two-phase equilibrium calculation, the following relationship must be satisfied:

$$T_{bp} < T_s < T_{dp}$$

Fig. 1

Continuous equilibrium flash fractionation



Nomenclature

E,F = Constants
K_i = Equilibrium flash constant for each component in the feed stream
L_i = Total moles of component i in the liquid phase
L = Total moles of liquid at equilibrium conditions
M_i = Total moles of component i in the feed stream
n_i = Mole fraction of component i in the feed stream
n = Number of components in the feed stream
R = Liquid-vapor (L/V) ratio (default value of $R = 1.0$)
R' = New L/V ratio for each iteration calculation
V = Total moles of vapor at equilibrium conditons
V_i = Total moles of component i in the vapor phase
X_i = Mole fraction of component i in the liquid phase
Y_i = Mole fraction of component i in the vapor phase