

Lecture 9

Equilibrium-based methods for multicomponent absorption, stripping, distillation, and extraction

Previously graphical, empirical, and approximate group methods for the solution of multi-stage separation problems involving equilibrium stages have been considered. Except for simple cases, such as binary distillation, these methods are suitable only for preliminary-design studies. Final design of multistage equipment for conducting multicomponent separations requires rigorous determination of temperatures, pressures, stream flow rates, stream compositions, and heat-transfer rates at each stage. (However, rigorous calculational procedures may not be justified when multicomponent physical properties or stage efficiencies are not well known.) This determination is made by solving material balance, energy balance, and equilibrium relations for each stage. Unfortunately, these relations are nonlinear algebraic equations that interact strongly. Consequently, solution procedures are relatively difficult and tedious. However, once the procedures are programmed for a high-speed digital computer, solutions are achieved fairly rapidly and almost routinely. Such programs are readily available and widely used. This lecture discusses the solution methods used by such programs, with applications to absorption, stripping, distillation, and liquid-liquid extraction. Applications to extractive, azeotropic, and reactive distillation are covered later.

This lecture begins with the development of a mathematical model for a general equilibrium stage for vapor-liquid contacting. The resulting equations, when collected together for a countercurrent cascade of stages, are often referred to as the MESH equations. A number of strategies for solving these equations have been proposed with those most important considered in detail here. All of these methods utilize an algorithm for solving a tridiagonal-matrix equation. When the feed(s) to the cascade contains components of a narrow boiling-point range, the bubble-point (BP) method is very efficient. When the components cover a wide range of volatilities, the sum-rates (SR) method is a better choice. The BP and SR methods are relatively simple, but are restricted to ideal and nearly ideal mixtures, and are limited in allowable specifications. There are more complex methods, Newton-Raphson (NR) and Inside-Out, respectively, which are required for nonideal systems. These two methods, which are widely available in process simulators such as ASPEN PLUS, CHEMCAD, HYSYS, and PRODI, also provide many specification options.

Consider a general, continuous, steady-state vapor-liquid or liquid-liquid separator consisting of a number of stages arranged in a countercurrent cascade. Assume that: (1) phase equilibrium is achieved at each stage, (2) no chemical reactions occur, and (3) entrainment of liquid drops in vapor and occlusion of vapor bubbles in liquid are negligible. A general schematic representation of an equilibrium stage j is shown in Figure 1 for a vapor-liquid separator, where the stages are numbered down from the top. The same representation applies to a liquid-liquid

separator if the higher density liquid phases are represented by liquid streams and the lower-density liquid phases are represented by vapor streams.

Entering stage j can be one single- or two-phase feed of molar flow rate F_j with overall composition in mole fractions $z_{i,j}$ of component i , temperature T_{Fj} pressure P_{Fj} , and corresponding overall molar enthalpy h_{Fj} . Feed pressure is assumed equal to or greater than stage pressure P_j . Any excess feed pressure ($P_f - P_j$) is reduced to zero adiabatically across valve F.

Also entering stage j can be interstage liquid from stage $j - 1$ above, if any, of molar flow rate L_{j-1} , with composition in mole fractions $x_{i,j-1}$, enthalpy h_{Lj-1} , temperature and pressure, which is equal to or less than the pressure of stage j . Pressure of liquid from stage $j - 1$ is increased adiabatically by hydrostatic head change across head L .

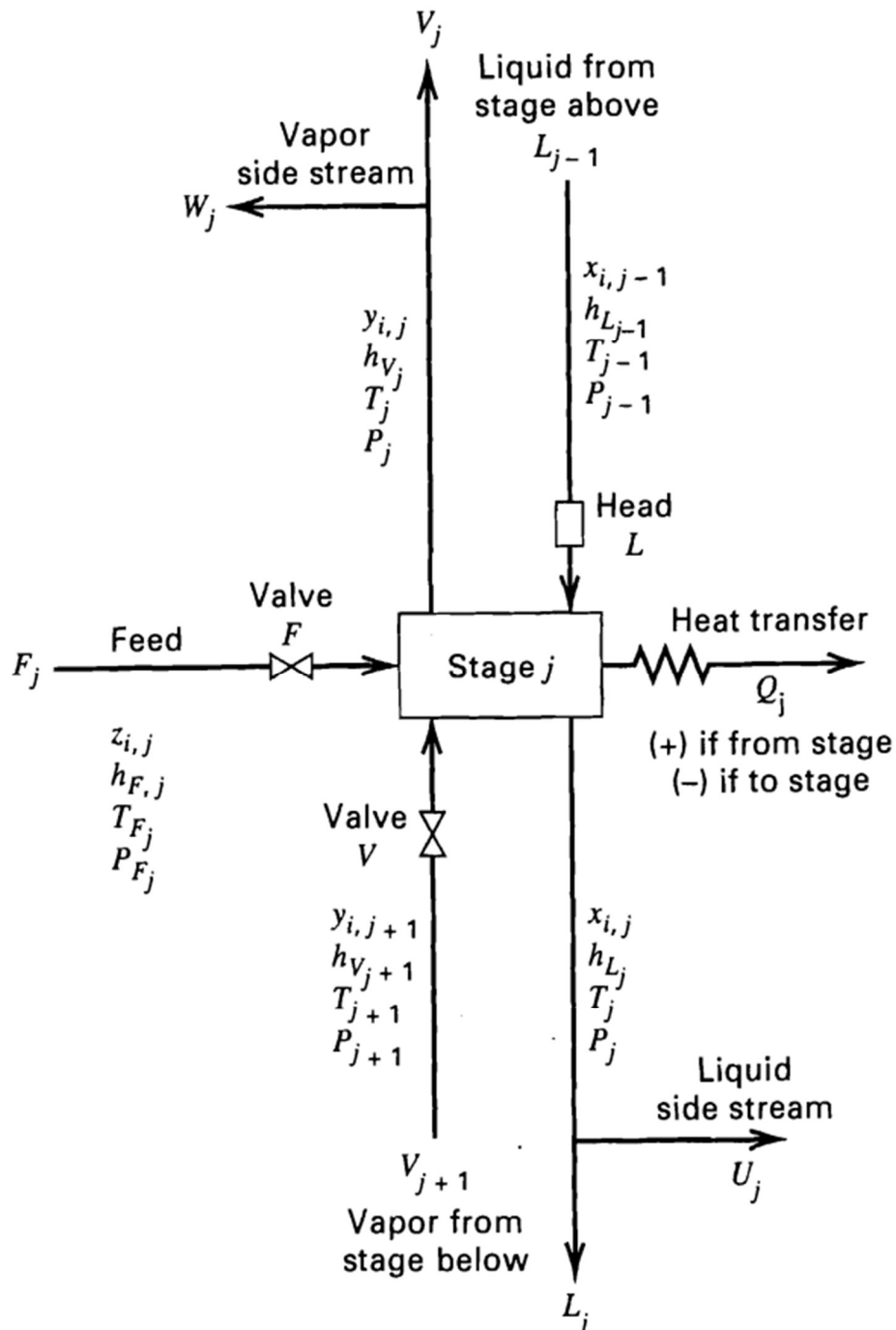


Figure 1 - General equilibrium stage