CHAPTER II

SURVEY OF THE LITERATURE

There are two basic approaches for analyzing the topping column. Simple but rather approximate, the first employs empirical correlations, e.g. those given by Packie (3) and Nelson (4), to relate the number of intervening stages to the degree of overlap of the boiling point curves for adjacent product streams. Watkins (5,6) used this approach to illustrate several examples representing different types of topping column. The approach works satisfactorily if the actual conditions are not too different from those on which the empirical correlations are based.

The second more exact approach adopts the concept of multicomponent distillation. The crude oil is conceptually divided into a sufficient number of pseudomulticomponents. Then numerical solution of the resulting multicomponent distillation is achieved using digital computers. In this chapter a survey of literature was conducted on these methods and the information gathered was utilized to improve the mathematical model and simulation procedure of topping column.

2.1 Rigorous Solutions of Multicomponent Distillation Problem

Initially, for the rigorous mathematical models of multicomponent distillation column, successive approximation procedures called convergence methods were developed and presented by Lyster et

al.(7-9) as the theta method for use in conjunction with the Thiele and Geddes procedure. To this method, Hardy et al.(10) added the constant composition arrangement of the enthalpy balance, and Holland (11) presented the K_b method for the evaluation of the new temperatures, and the constant-composition method for solving the enthalpy balances for the total-flow rates. Friday and Smith (12) gave a summary of the concepts and problems associated with the iterative methods. Originally, the material balances were solved by nesting procedures. Boynton's technique (13) used the inner and outer loop convergence to determine a set of phase flows and temperatures which satisfy both material and energy balances. More recently, matrix techniques have been employed, in which the material balances are stated in tridiagonal form. Present formulations of the theta method as given by Holland (2,14) incorporate these matrices.

The multicomponent distillation problem was formulated as the solution to a set of nonlinear simultaneous equations by Amundson and Pontinen (15). For distillation and adsorption, the most general formulation involves $N(2c + 3)$ equations and variables, where N is the number of equilibrium stages, and c is the number of components. Most of the solution algorithms use the Newton-Raphson method as part of an iterative process solving either a subset or the complete set of equations. Greendstadt et al (16) were among the first to apply the Newton-Raphson method to the solution of distillation problems. In 1961, Sujata (17) proposed an approximate application of the Newton-Raphson method for the solution of absorber and stripper pro-blems. Sujata regarded the temperatures as the independent variables. For each set of assumed temperatures, the component material balances

and equilibrium relationships were solved by direct iteration for the solution sets of compositions and flow rates. These compositions and flow rates were then used in the enthalpy balances in the calculation of an improved set of temperatures by use of the Newton-Raphson method. In Sujata's application of the Newton-Raphson method to the enthalpy balances, the dependency of the flow rates and compositions on the temperature was neglected in the calculation of the partial derivatives. A version of the theta method, called the " single-θ-method " has been proposed (2).

Another formulation of the Newton-Raphson method was proposed by Newman (18) in 1963 in which the total liquid flow rates were taken as the independent variables and the corresponding sets of temperatures needed to satisfy the component material balances and equilibrium relationships was found by successive application of the Newton-Raphson equations. The compositions and temperatures so obtained were used to solve the enthalpy balances explicitly for a new set of liquid flow rates. The procedure was then repeated by commencing with this most recent set of liquid flow rates.

Following Newman, Boynton (13) also took the liquid flow rates to be the independent variables, and for each choice of these variables the temperatures required to satisfy the component-material balances and equilibrium relationships were found by successive application of the Newton-Raphson method. The results so obtained were then used in the enthalpy balances to compute a new set of liquid rates by use of one application of the Newton-Raphson method. For the case where both the vapor and liquid phases form ideal solutions, the Boynton's method constitutes an exact application of

the Newton-Raphson method. All of the matrix equations solved by Boynton were of order N.

Another exact formulation of the Newton-Raphson method, called the multiple theta (multi-θ) method, was proposed by Holland (2). However, it will be called the 2N-Newton-Raphson formulation to distinguish it from other solution methods. Two procedures for applying this method were presented. In both of the procedures, the matrices were all of order N. All derivatives were evaluated by use of the calculus of matrices.

Tierney and Bruno (19) proposed an application of the Newton-Raphson method in which the vapor rate and the temperature of each stage were taken to be independent variables. The Jacobian matrix was evaluated analytically by Tierney and Yanosik (20) with the same choice of independent variables. In their analysis, they observed a near constant Jacobian matrix close to the solution region. Then, in order to reduce computational effort, Orbach et al.(21) evaluated the Jacobian numerically, computed its inverse, and held it fixed for several iterations. Tomich (22) proposed a quasi-Newton method using Broyden's matrix update formula to approximate changes to the Jacobian inverse from changes made to the variables and changes resulting in the errors.

Hutchison and Shewchuk (23) also presented an alternated arrangement of the equations for distillation which utilized the insensitivity of relative volatilities and developed the enthalpy equations in terms of the activity coefficients in such a way that made the computation efficient for regular solutions. Boston-Sullivan algorithm (24) is based on the use of newly defined energy and vola-

tility parameters as the primary successive approximation variables, and Broyden's method is used to iterate on these parameters. Holland (2) gives a method for using " virtual " values of the partial molar enthalpy for obtaining enthalpies of mixtures. Fredenslund et al. (25,26) discuss combination of the full multivariate Newton solution with the UNIFAC method for predicting activity coefficients and vapor-liquid equilibrium. Fredenslund et al. (26) also give a full listing of the computer program for such calculations. A simpler program using simultaneous convergence with less complex equilibrium expressions has been shown in Ref.(27).

T-method, a new convergence promoter was presented by Pierucciet al.(28), in which the feed tray temperatures are manipulated to account for the differences of chemical components. Kaufmann and Montalvo (29) described the application of a modified damped Newton method in 1983, which incorporated the feature that a monotonic convergence toward the solution was always achieved. The modifications included the determination of the appropriate search direction (possibly opposite to Newton's search direction) and the step size in such a way that a monotonic convergence toward the solution was assured. Most recently, Yamada et al.(30) proposed E^V-matrix method which used the vaporization plate efficiency. This new method has a concise algorithm, similar to that of Amundson and Pontinen but it also takes in account liquid entrainment from the plates and partial vapor condensation due to heat loss through the column wall.

2.2 Solutions of Crude Distillation Problem

Most of the rigorous solutions of multicomponent distillation

problem have limitations when applied to crude distillation problem. Some may be specific to a certain type of column. Others may be suitable for small columns, but when applied to large column require excessive computer time or fail to converge. In many cases, good initial estimates of temperatures and flow profiles are required. Another shortcoming is the inability of a program to satisfy realistic specifications, such as product quality or flow units.

The formulation of multicomponent distillation was first modified for calculating crude oil topping column by Prater and Boyd in 1955 (31). The proposed method of calculation was based upon a true-boling-point (TBP) analysis which divided the crude oil into desired number of pseudocomponents corresponding to normal paraffinic hydrocarbons boiling within these temperature ranges. The resulting information was used in the design of a multidraw crude oil topping column by combining of the Fenske method for obtaining the minimum number of trays at total reflux, the Scheibel-Montross method for calculating minimum reflux with an infinite number of plates, and the Gilliland correlation between reflux rate and number of theoretical trays. Van Winkle (32) outlined the calculational procedure for complex mixtures, such as crude oil, similar to that of Prater and Boyd.

Dickey et al. (33) proposed a calculational method for distillation with a sidestripper which can be applied to the crude oil topping column. The sidestripper was solved in the same convergence loop as the primary distillation column to obtain simultaneous convergence of these two units. The calculational procedure used the method of Thiele and Geddes (34) and the Θ-method of convergence.

Thus the stripper was in effect is considered as part of the distillation column. This procedure differed from the one adopted by Amundson et al. (35) in which they obtained solutions alternately for the distillation column and the sidestripper.

Gilbert et al. (36) and Jacob (37) presented a means of using a fractionation index to predict TBP data for the products from a crude oil distillation column. The value of the fractionation index is readily calculated using the Fenske-Underwood equation when component analyses of the feed and products are available. They also presented a method for treating the product TBP curves as algebraic functions without the necessity to break the feed TBP data into arbitrary pseudomulticomponents. The fractionation index can be derived directly from the product TBP data, or the TBP data can be calculated when the fractionation index is known.

Hariu and Sage (38) estimated the equilibrium flash vaporization of crude oil with the aid of a computer and showed several correlations to predict the pseudocomponent properties.

Formulation of the Newton-Raphson method was first applied to solve a crude topping column problem involving a system of columns in 1963 by Cecchetti et al. (39). He demonstrated the approach by use of the original-θ-method of convergence. In this procedure, the crude was characterized by pseudomulticomponents. The physical properties (normal boiling points, densities, and molecular weights) of the 34 pseudocomponents used to represent the TBP curves of the feed, distillate,and sidestreams are presented and each pseudocomponent is described by a set of vapor-liquid equilibrium K-values and a set of vapor and liquid enthalpies. The temperature, vapor and liquid rate

profiles are the independent variables. On the basis of assumed profiles, the calculations may be carried out from the condenser down and from the last stage up to the feed plate. At the feed plate, the results of these calculations are combined to give the compositions of the terminal products. The calculated values of the terminal rates are corrected by use of the O-method of convergence. The corrected molal withdrawal rates of components in the distillate and bottom products are used in the calculation of the compositions for each plate. An improved temperature profile is determined on the basis of these compositions. Improved liquid and vapor rates throughout the column are computed by use of enthalpy balances. In the evaluation of the enthalpies of the liquid and vapor streams, the improved compositions and temperatures are employed.

Cecchetti et al. (39) found a theoretical analogue column by trial. The theoretical analogue column is defined as one having perfect plates that gives calculated results in good agreement with field test results. The theoretical analogue column was restudied by Hess et al. (40) who regarded water as being distributed between the vapor and liquid phases on main stages, whereas Cecchetti et al. regarded water to be present only in the vapor phase on these stages.

Hess et al. used the temperature and liquid-to-vapor ratio of each stage as independent variables. The number of independent variables was equal to 2N+1 because the existence of two liquid phases in the accumulator gave rise to three independent variables for the first stage. The multi-θ-method or 2N+1-Newton-Raphson was introduced to solve the 2N+1 independent equations comprising the N+1 equilibrium relationships and the N enthalpy balances in functional

form.   Hess et al. demonstrated the use of three efficient numerical procedures for solving topping column problems. The first procedure was based on the evaluation of the derivatives in the Newton-Raphson equations by means of analytical expressions. The second and third procedures were based on numerical approximation of the derivatives by means use of the corresponding difference equations.