CHAPTER II

LITERATURE REVIEW

Shacham, M., Nacchietto, S., Stutzman L. F., and Babcock P. (1982) suggested that an Equation Oriented (EO) should be used to solve for small process flowsheeting problems, its implementation for large scale optimization or design problems would require developments of technology, mainly in the following areas: the verification of the input data, the ordering of the equations for solution, the initialization of the vector of the unknowns, and the development of a standardized thermodynamic interface. The programs ASCEND (Carnegie Mellon University), FLOWSIM (University of Connecticut) and SPEEDUP (Imperial College) are in the most advanced state of developments.

Pierucci, S., Troiani, F., Ranzi, E., and Biardi, G. (1982) solved countercurrent separation units by the combination of two models referred to the sure and the fast models. The sure model was employed for trays having particular feature, or disturbances, i. e. feed trays, partial condenser, reboilers, side cuts, intercooler, ect. as well as for tray adjacent to the previous ones. This model was written in terms of single theoretical tray equations. The fast model was applied to multitray sections, provided that no disturbance exists. A Newton-Raphson procedure, combined with a BP method, was employed to converge the set of equations describing the problems. This model was shown in figure 2-1.

The results agreed well with those obtained by rigorous tray-by-tray calculations. The computing time has become shorter because the effective number of trays has been reduced.

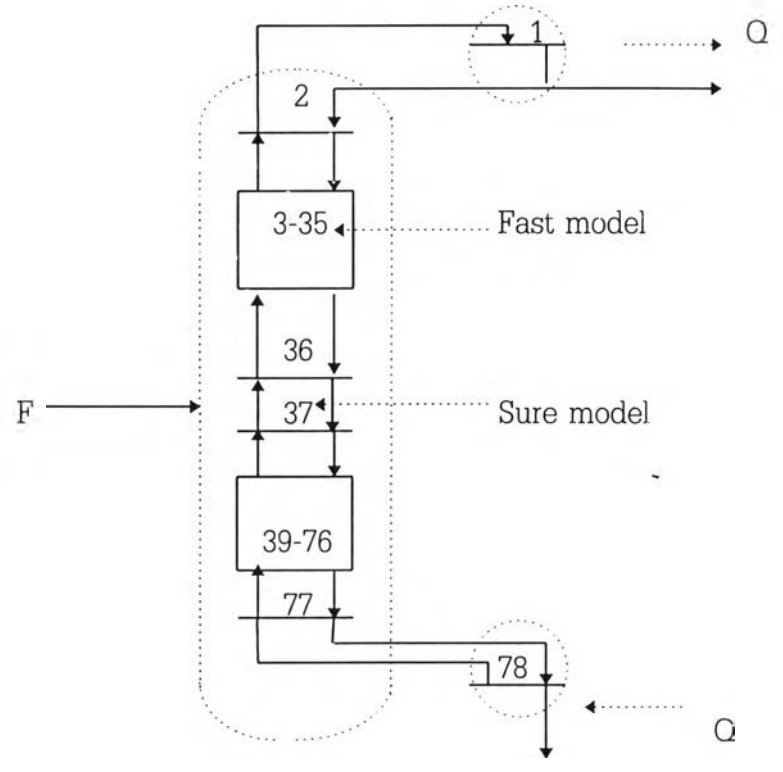

Figure 2-1 The combining sure and fast model.

Gundersen T. (1982) presented the failures in flash calculations ($K_i \rightarrow 1.0$) when cubic equations of state, Soave modified Redlich-Kwong and Peng-Robinson equations, were used to estimate equilibrium K-values. It still has had two main deficiencies. One is the well-known problem of guessing good starting values of the phase compositions at high pressure. The other is that regular method for soling the cubic equation in the compressibility often lead to a wrong type of roots (i.e. vapor and liquid).

S. Venkataraman and A. Lucia (1988) solved the distillation problems by Newton-like methods. A generic initialization procedure makes some certain Newton-like methods very reliable. The Thermodynamically consistent hybrid method is more efficient than Newton's method with analytical derivatives and

conditions under which line searching and dogleg strategies expand domains of attraction were identified.

Vazquez-Esparragoza, J. J., McLaughlin, B. E., Naugle N. W., and Holland C. D. (1988) used the combination of the functional transformation and the Newton-Raphson methods to solve distillation problems which were either difficult or impossible to solve by using only the Newton-Raphson method. The functional transformation method was applied to large systems of nonlinear equations by Vazquez-Esparragoza.

Seader J. D. (1989) suggested that the rate-based model and the accompanying algorithm for implementing it with a digital computer was the harold of the design and simulation of tray-tray separators. The rate-based approach avoided the uncertainties of tray efficiencies, and it provided a model based on mass, heat, and momentum transfer fundamentals and was particularly recommended for nonideal multicomponent system. It was useful even for nearly ideal multicomponent systems when good predictions of product distributions were desired for components other than the key components.

Colussi, I.E., Fermeglia, M., Gallo, V., and Kikic, I. (1992) developed program GLOBUS combining a rigorous method for column solving (simultaneous convergence method) to a rigorous thermodynamic routine. It showed its reliability for simulation of supercritical and near-critical multistage multicomponent extraction columns, provided that the given chemical system was well-described by the thermodynamic model used.

Onana, A. and Hikolo, A. M. (1993) used a successive over-relaxation (SOR) method for computations of multicomponent equilibrium stage separation operation. They demonstrated the efficiency of iterative methods using numerical comparisons, covering a wide range of number of components and number of stages. It showed that the SOR method was more efficient than the Thomas algorithm when the number of components was large.

Wilhelm, C. E., and Swaney, R. E. (1994) presented a robust solution method for the large-scale, structured sparse nonlinear algebraic equation system involved in steady-state process modeling calculations. The strategy progressively invoked more involved computations was able to solve linear programs that combine local Jacobian and global bounding information to generate corrected search directions and to assess region feasibility. Interval analysis techniques were employed to automatically generate bounding functions from the analytical expressions for the equations. Adaptive domain partitioning together with a branch and a bound structures provided a formal backtracking mechanism.

Thanit Sawasdisevi (1996) developed a database system for searching and estimating properties of gas and liquid. The database developed by C++ language contained 150 components. Ideal gas, Soave Redlich Kwong, and Peng-Robinson models were employed to predict vapor-liquid equilibrium.