CHAPTER II

SURVEY OF THE LITERATURE

The calculation of multicomponent separation in complex columns such as reboiled absorbers and multi-feed, multi-sidedraw fractionators, has become more and more important in modern process design. Efforts to computerize rigorous separation calculations may be classified into the following two categories:

Type A Methods. Computer solutions were obtained for the plate-to-plate calculation procedures, namely, the Lewis-Matheson method and the Thiele-Geddes method, developed in the thirties. Aronofsky, Bonner, Hanson, McIntire and Shelton, among others, applied the Lewis-Matheson method on computers for the calculation of conventional fractionators. Bard and Greenstadt employed the Newton-Raphson method for the simultaneous solution of the system of equations used in the Lewis-Metheson method. These method worked for both conventional and complex columns. Holland and coworkers develop a "θ-method" to couple with the method of Thiele and Geddes for handling both conventional and complex columns. A Service Bureau Corp. computer program used a method similar to that of Holland's . Hopper and Bailey then modified the "θ-method" by combining it with the fraction index concept of Geddes.

Type B Method. The rigorous computational procedures were developed for the simultaneous solution of the system of equations. Examples of this type are: Amundson's matrix method, the Relaxation method of Ball and Rose, Naphthali's method, and the method of Wang and Oleson.

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Friday and Smith gave an excellent analysis for the equilibrium stage separation problems. They concluded:

* Type A methods are numerically unstable and thus are basically unsuited for computer calculation of complex columns with multiple feeds and multiple side streams.

* Type B methods are not susceptible to important round-off errors and work equally well for any number of feed and side streams.

All the previous type B methods, however, either are too slow (the relaxation method and the Wang-Oleson method). Furthermore, most of these method use the Newton-Raphson method for convergence. There is generally no assurance that the Newton-Raphson method would converge. Consequently, there has no been wirespread application of type B methods. J.C. Wang and G.E. Henke developed a new computational procedure to make the type B method more attractive. A tridiagonal matrix method is developed.

Phase equilibrium computations for mixtures containing heavy hydrocarbon fractions are usually regarded as being difficult and mysterious, somewhat reminiscent of the methods of the alchemists. Lack of experimental data for these mixtures and the necessity of representing the highly complex heavy fractions by means of relatively few model compounds or parameters are some of the main reasons for this. The difficulties of representing complex hydrocarbon mixtures have resulted in simulation procedures where the EOS parameters are adjusted to match the saturation points (Coats and Smart, 1982; Whitson, 1982; Wilson et al., 1978). Karen Schou Pedersen, Per Thomassen, and Aage Fredenslund has been develop a purely predictive method and described phase envelop calculations. A phase envelop program (TERM) has been developed by Michelsen (1980,1982). The program can

treat mixtures of H_2O, N_2, CO_2, H_2S, and hydrocarbons from C_1 to C_9. This program has been extended to mixtures containing hydrocarbons heavier than C_9. The vapor-liquid equilibria are represented in TERM by either the Soave-Redlich-Kwong (Soave, 1972) or the Peng-Robinson (1976) equations of state.

The necessary input parameters are a critical temperature and pressure and an acentric factor for each component and a binary interaction parameter between each pair of components. Acentric factors and critical properties of each subfraction have then been estimated from specific gravity, molecular weight, and boiling points using different correlations.