CHAPTER VI

DISCUSSION

6.1 Development of simulator

The distillation model used for this simulator consists of a series of equilibrium stage as discussed in chapter III. It is suitable to model the complex column which has many feed streams, vapor or liquid sidestreams and side exchangers. The equilibrium stage used in this simulator can be used to model another stage separator such as absorber and stripper, also. The further study on this simulator program can be conducted modify to solve absorption and stripping problem.

The calculation procedure using bubble-point (BP) method is the rigorous method which can provide exact solution limited only by accuracy of the phase-equilibrium and enthalpy data utilized. [Henry, E. J., 1981] The tridiagonal matrix consisting of arrays of variables is used in this technique. Firstly, it requires high memory to run this problem. This personal computer had not enough memory to manage the problem in first time. The problem of memory can finally be solved by using a dynamic array which is the key of C++ programming. The database program developed by C++ is linked to this simulator. It is used to estimate bubble-point temperature, phase equilibrium constants and enthalpy of streams.

The simulator developed by C++ language has a lot of graphic user interfaces designed to be friendly to user. It is convenient to input all of the required data to solve distillation problems. There are two steps to input data.

First, the simulator will show a window for input the column configurations, and then it will show automatically another window for selecting components when user has finished input. The second step, the user can select a input window from menu or click on any active area of the figure of conventional column on the main window. The simulator offers several selection of property methods, including Ideal Gas, Peng-Robinson and Soave Redlich Kwong. It consists of several unit systems of temperature, pressure, flowrates and energy flows which can be selected by users. It is easy to input and change values of any data in the input windows. The input data can be checked before starting calculation using the commands available on the command menu. The program will show the warning message when it finds the incomplete data.

Help files of simulator can be used to help users to start the simulator easily. The help file provides suggestion as follows.

- How to use this simulator.
- How to input data.
- Description of warning messages displayed on screen
- About distillation simulator.

The results of calculation will be shown on window that selected from "Report" menu. The output are displayed in table form and temperature profiles shown in the graphic form.

6.2 Program verification

The output from simulator are checked by material balance of the column. The material balance relative errors of all the cases discussed in chapter V. The maximum error occurred is ±3.39%. Because the equations of state available in this simulator can provide moderate accurate for the polar compounds. The error in the condenser and reboiler have small value but they seem to be large in some certain stages of the column. It may be taken place by the energy balance equation used to determinate vapor and liquid interstage flowrate. The error of total material balance in each tray are found to be nearly zero.

The results of calculation using the PR model have the error less than those of the SRK model when the system contains non-polar compounds. For the polar compounds system, users should select the SRK model to estimate properties. It can predict better than the PR model.

The results of calculation are compared to the reference data. The temperature and liquid composition profiles are considered. The temperature profiles obtained using the simulator and those from reference data have similar shape. The maximum differences are ±0.46% for the results using the PR model and ±0.31% for SRK model. The liquid composition relative difference using the PR model is -63.94%. Benzene, which is the light component in this system, has low composition in reboiler as 0.002951 which is different, -0.001151, from the reference. It has maximum difference using the PR model as ±1.39 in rectifying section. Similarly, the results using the SRK model has -34.97% as maximum and ±1.06% as the maximum relative difference in the rectifying section. In this case, the simulator has comparatively large difference from reference data in rectifying section when the component is the heavy key. Similarly, the high relative values which are compared to reference data occurred in the stripping section for the light components.

Considering the comparison to the commercial simulator named HYSIM, the profiles of temperature, liquid and vapor composition obtained from the simulator and HYSIM are similar. The differences seem to be small when they are considered as absolute values but they are large when compared to HYSIM as the relative difference. The relative differences have occurred in the column has the same reasons as comparison to the reference data. The light component has large difference in stripping section which contains low composition and the heavy component has large difference in rectifying section.

The results of simulation are differents due to tolerance is changed. The maximum error using 0.01N as the tolerance is 0.0613%.

6.3 Distillation simulations

Distillation calculation is also too difficult and too complicated to solve manually. Users can use this simulator to solve the distillation case which the operating conditions can be changed. The outputs of the simulation can be compared to basic cases. For example, a case of conventional distillation column is compared to a more complicated one which has many feed streams, side exchangers, vapor or liquid sidestreams. This simulator is convenient to change the operating conditions (i. e. feed conditions, reflux ratio, column configurations, pressure, top and bottom product). Users can use the results of both cases to study behavior in the column. The considered characteristics shown in the output of simulator are temperature, vapor and liquid composition profiles, heat duties and purity of products. The purity of products can become better or becomes worse than that of the previous case depending on the conditions considered. The energy consumption is also similar to the value of purity. The results of simulation can help users to find the suitable operating conditions.

The simulator can also be used to checked basic design of distillation column. The basic design calculated by approximating method provides number of stages, feed trays, reflux ratio and another operating conditions. Users can input the designed data into the simulator. The results of simulator are compared to column specifications.

The study and experiment on distillation column in both pilot scale and plant scale require very high costs and consume a lot of energy. Therefore, this simulator is very useful for students and operators to use it for studying the distillation.

6.4 Limitation of simulator

This simulator requires high memories for solving distillation problems. It is tested on personal computer which has 486DX2 microprocessor with 8MB RAM. It can solve the problems of distillation columns which have maximum stages of 40. The number of components is less important than the number of stages since it effects to the memories required in comparison with the number of stages.