CHAPTER IV

DEVELOPMENT OF THE SIMULATOR

4.1 Computer Program of Distillation Calculation

The program developed by using C^{++} language could be run under Microsoft Windows version 3.1 or later. The personal computer which have at least 386DX microprocessor with 4 MB RAM and VGA monitor could be run this simulator. The 486 DX2 with 8MB RAM is recommended. This simulator is composed of four parts as follows,

4.1.1 Input Data

Base on chapter III, the rigorous model that requires a lot of input data is chosen in this work. The input data required for solving distillation problems are difficult to enter them into computer program due to its complexity. Then, the input tools are developed to enter the data easily. The details of input dialogs are shown as follows:

1) Components selection

Users can select components in the list which is shown on this dialog. It allows the user to select the maximum number of components up to 10. The warning message is automatically shown when the list of selected components is changed. The selection of components must be done otherwise

other parts of program cannot be run before selecting components. (refer to figure 4.1)

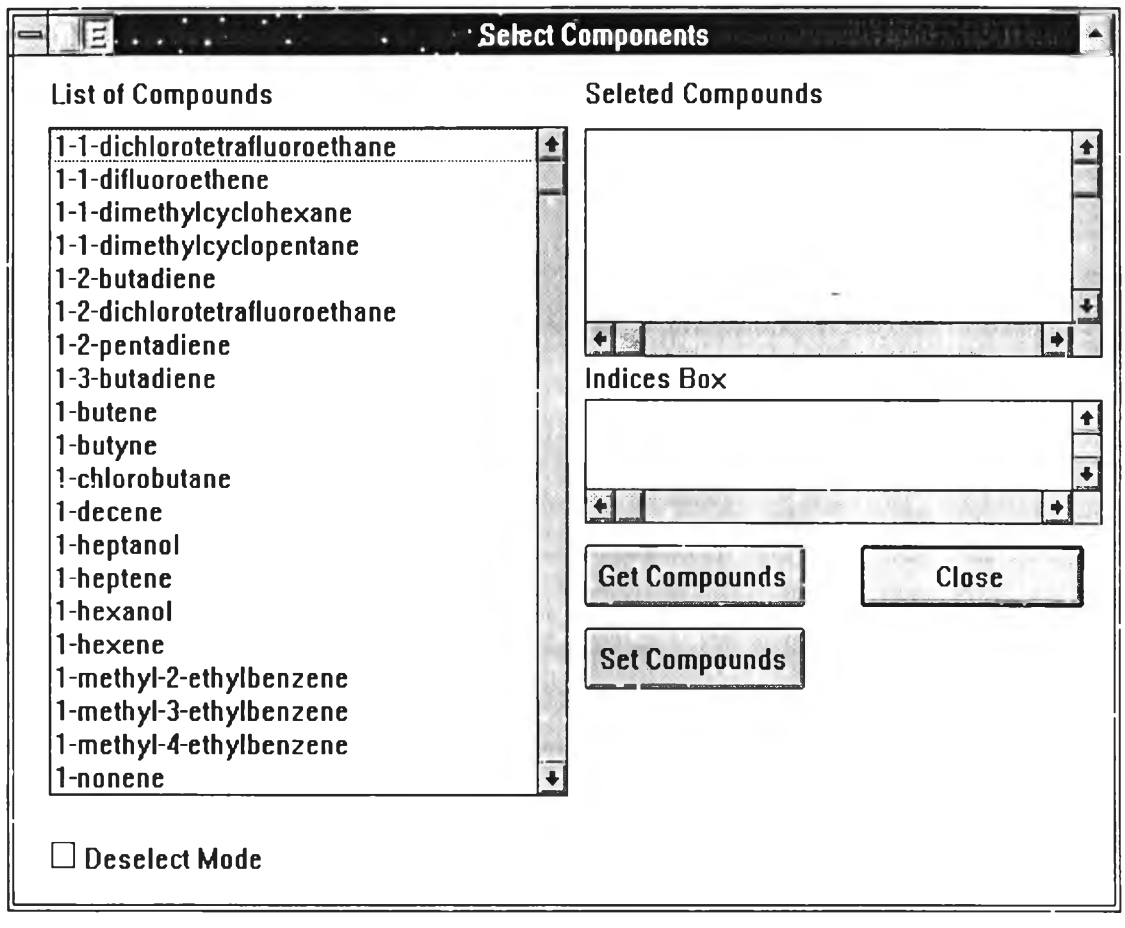

Figure 4.1 The Dialog for selecting component.

2) Selection of thermodynamic property models

Thermodynamic properties of vapor and liquid are estimated from one of three model, namely Ideal gas, Soave Redlich Kwong and Peng-Robinson models. Users can select the appropriate model from menu item "Properties package" in the Select menu. The PR is a default of this program.

3) Column configurations selection

Users have to specify the column configurations, including

- the number of stages
- the number of feeds
- the number of side streams
- the number of energy streams (Side exchanger)
- reflux ratio

The maximum number of stages is up to 100. It is illustrated in figure 4.2.

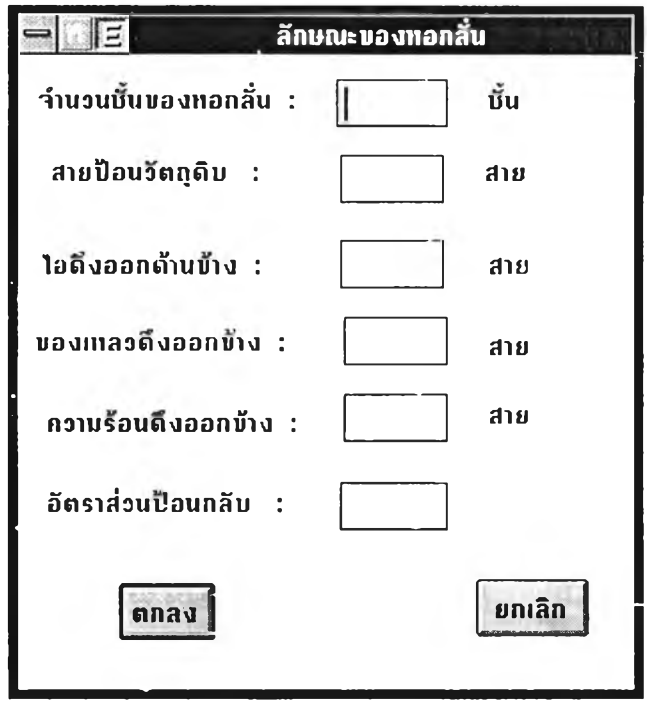

Figure 4.2 The Column Configuration dialog

4) Feed dialog determination

The operating condition of feed must be specified in this dialog are the feed temperature, pressure, flowrate with the composition, and the location of feed stream. This dialog is shown in figure 4.3.

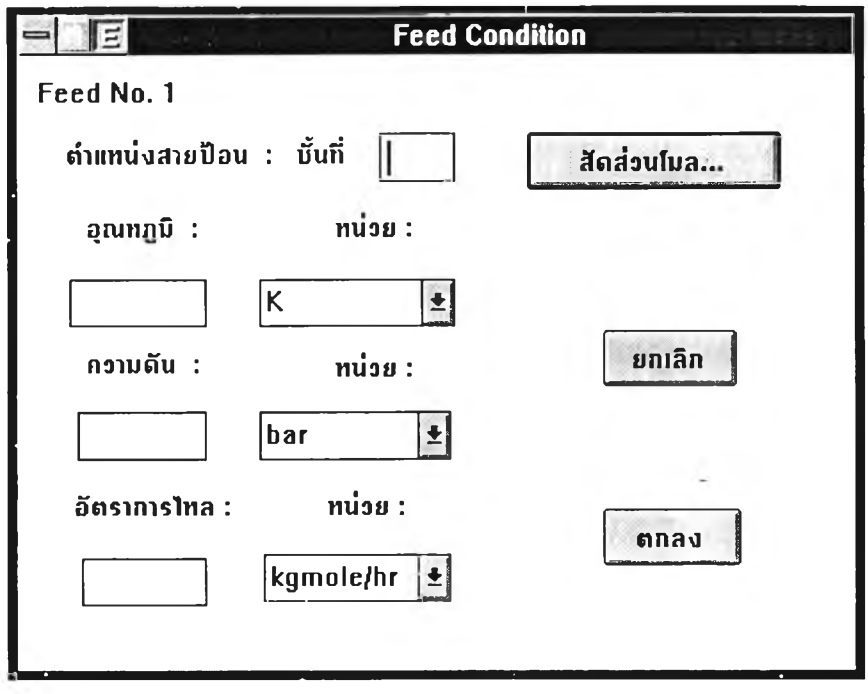

Figure 4.3 The Feed Dialog

Users can call this dialog from the command menu or the active area of Feed in schematic diagram shown in the main window Users can input feed composition of each component in the dialog which is displayed when the "สัดส่วนโมล..." button is clicked. The dialog is shown in figure 4.4

Users may input molar flowrate for each component. This program will normalize the molar composition after the "ตกลง" button is clicked.

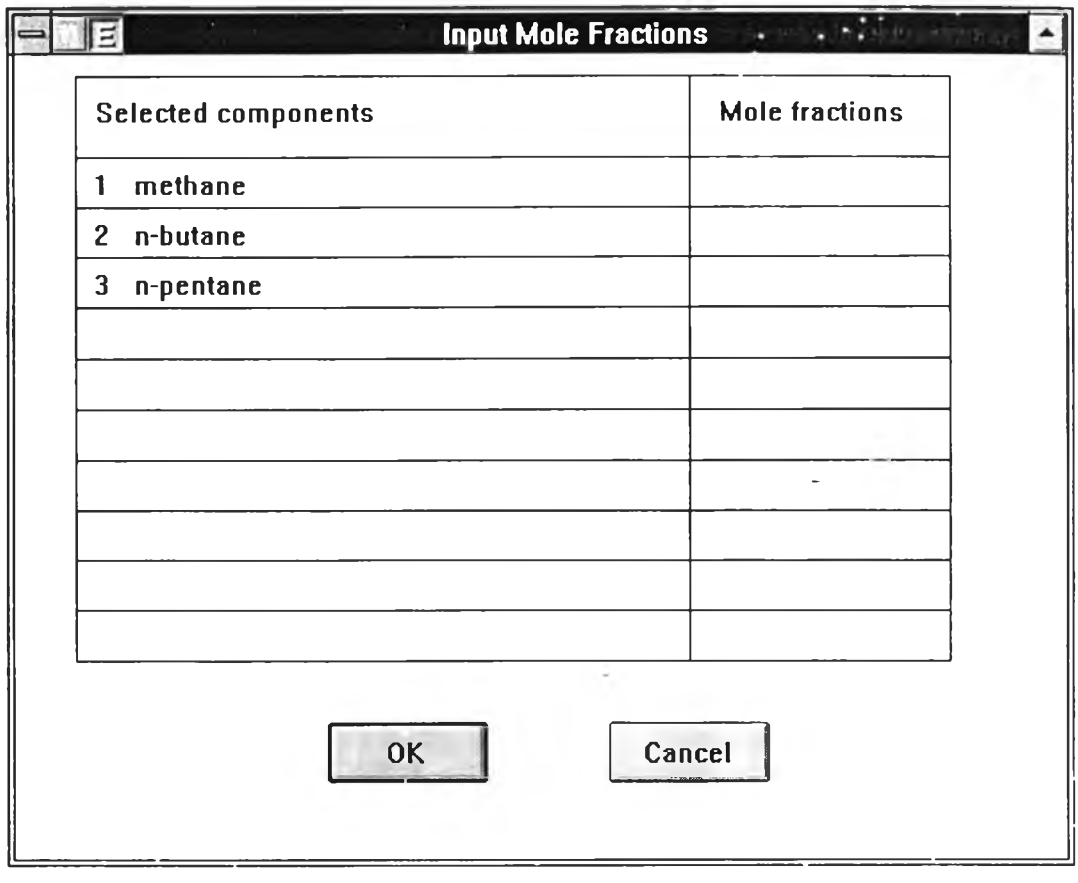

Figure 4.4 The Dialog for input feed composition.

5) Vapor/ Liquid top product determination

Users select this dialog from the command menu or activate it by double clicking on the top product stream in the schematic diagram of distillation column. The data entered into the program consist of temperature, pressure and flowrate. There are two kinds of probable product which is liquid or vapor, depending on the condition of temperature and pressure. The dialog is shown in figure 4.5.

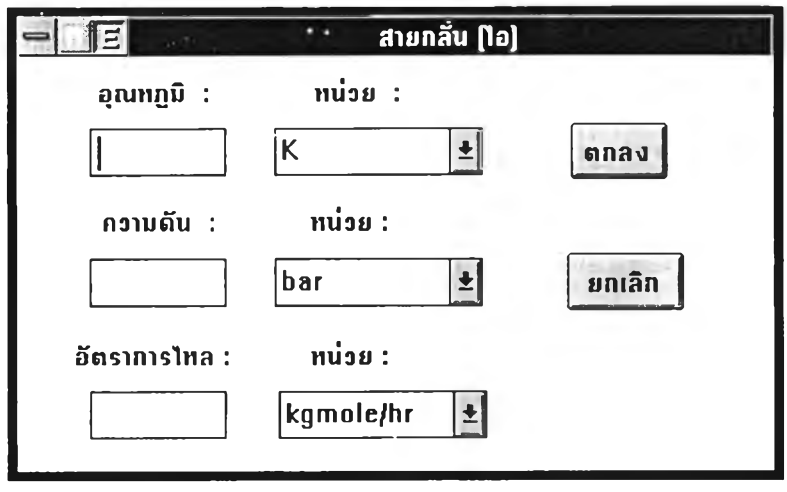

Figure 4.5 The Top Product Dialog

6) Bottom product determination

This dialog is similar to the top product as shown in figure 4.6. The bottom product (สายก้นหอ) is liquid side stream from reboiler with flowrate which can be determinated by this program.

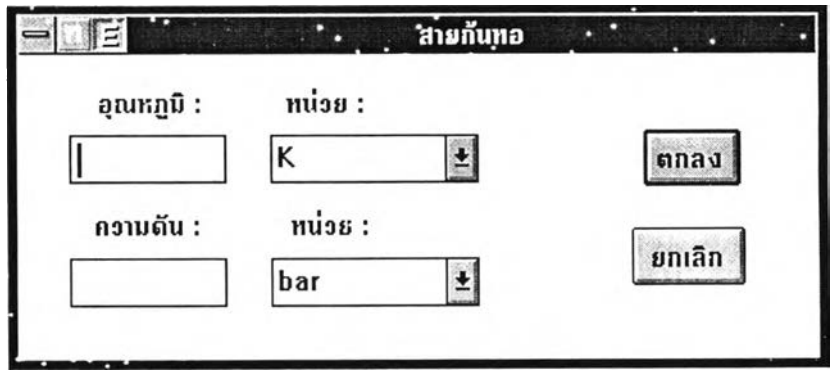

Figure 4.6. The Bottom Product Dialog

7) Vapor/Liquid side stream determination

A dialog for determining the side stream data which consists of flowrate and location of each stream can be chosen from Edit menu. It is convenient to input data in the dialog as illustrated in figure 4.7.

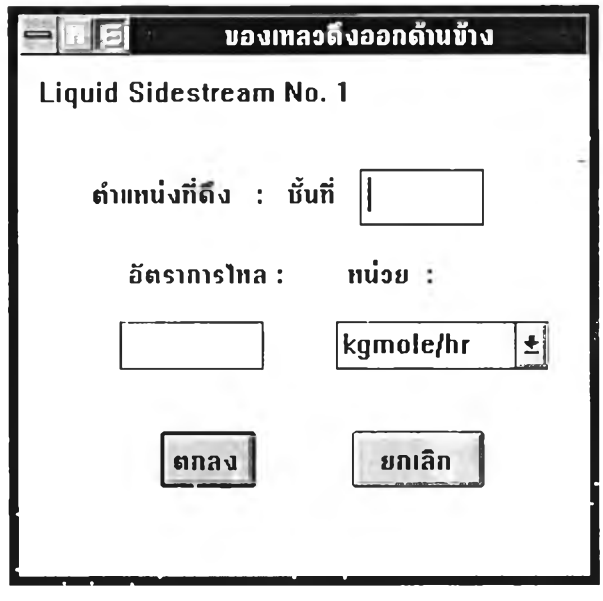

Figure 4.7 The Side Stream Dialog

8) Determining of heat transfer to/from each stage

Data of the heat transfer to or from each stage consist of as heat transfer rate and it's location User have to enter heat transfer rates to or from all individual stages except stage 1 (condenser) and stage N (reboiler).

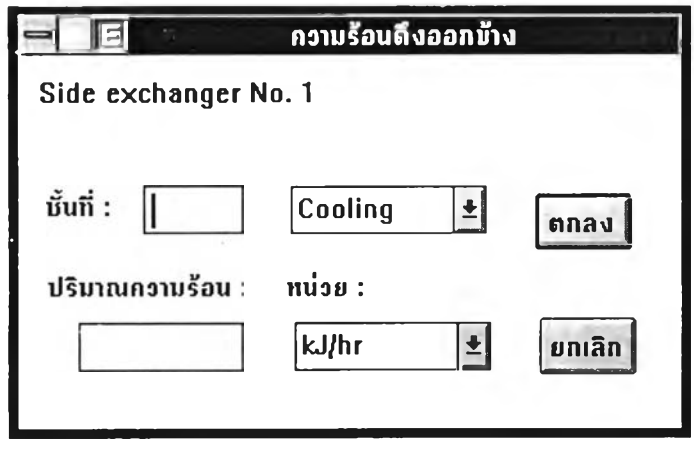

Figure 4.8 The Dialog for Entering Heat Transfer Data

Before running this program, it is recommended to check the input data from menu item "Check Input" presented in Report menu. However, the data can be changed by selecting the input dialog and entering new data in the dialog of the data which users want to change.

Table 4.1 summarizes the input data that must be input into this program.

Table 4.1 Summary of Input Data

Input Data	Details of Input Data
Mixture	Component
Column Configurations	The number of stages
	The number of feeds
	The number of side streams
	The number of heat transfer rates
	Reflux ratio
Feed	Feed location
	Flowrate
	Temperature
	Pressure
Product	
- Vapor top product	Flowrate
- Liquid top product	Temperature
- Bottom product	Pressure
Side streams	
- Vapor side streams	Flowrate
- Liquid side streams	Stream location
Heat transfer rate to or	
from stage	Heat transfer rates
	Stream locations

4.1.2 Database

This program is linked to the database developed by using C^{++} language. Thermodynamic properties and vapor-liquid equilibrium shown in chapter III can be calculated using data from the database and are sent to the calculation module, for solving the distillation problem.

Users have to select the model for estimating the thermodynamic properties of all components. For a nonideal case, Soave Redlich Kwong or Peng-Robinson will be used for calculating the properties.

4.1.3 Computational Procedure

The computational procedure used in this program was modified from Boiling Point method. The details of development was discussed in 4.2.

4.1.4 Output

The results of calculation are presented in tabular form which is displayed on Windows. Two windows show the results of simulation. The first window exhibits temperature, pressure, flowrate with the composition of each component, and enthalpies of vapor-liquid sidestreams, vapor-liquid top products and bottom products, see figure 4.9. The other displays temperature, pressure, and composition distribution in the column, figure 4.12. In addition, figure 4.13 presents the temperature distribution with respect to the equilibrium stages.

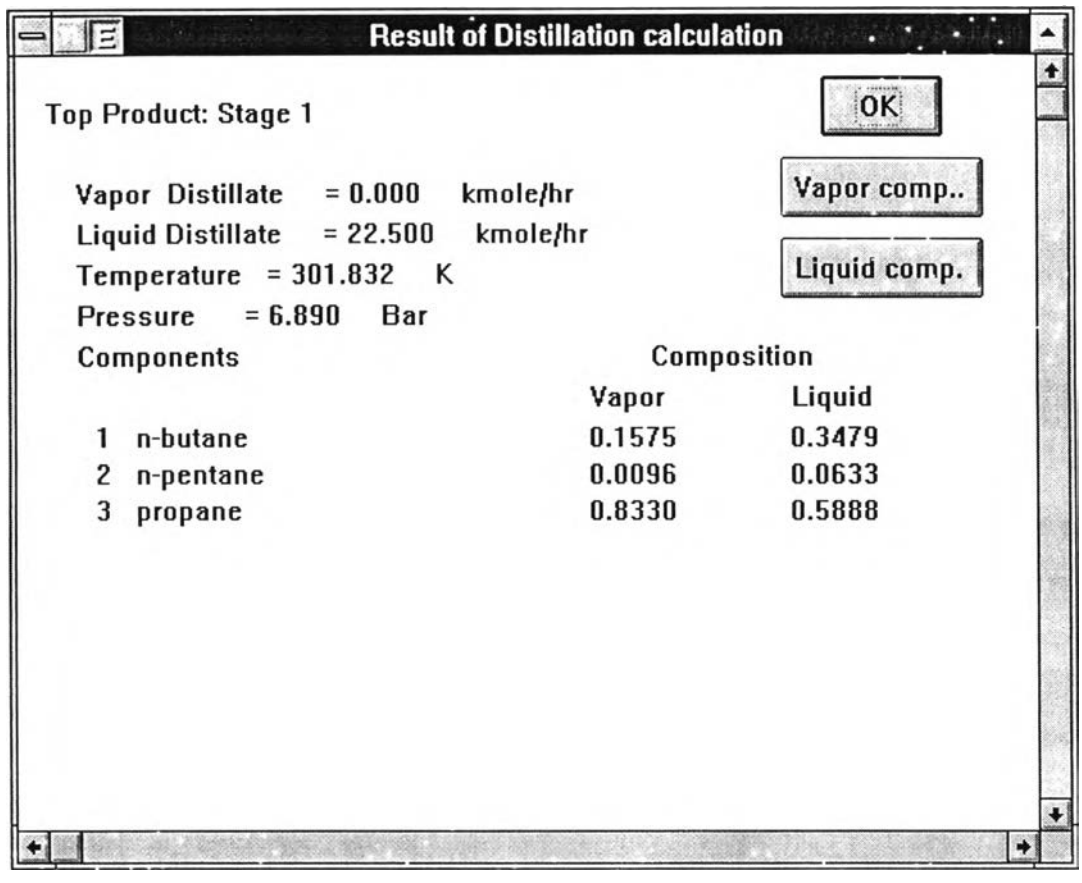

Figure 4.9 The output window

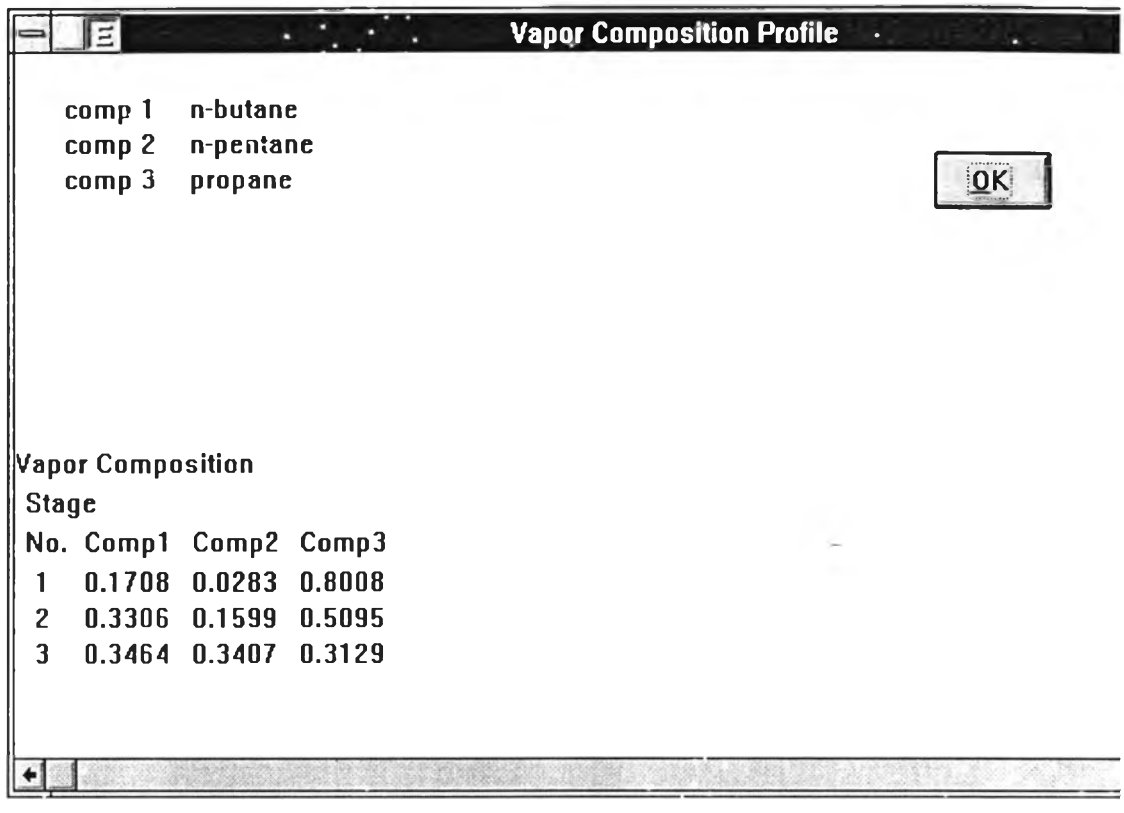

Figure 4.10 The vapor composition window.

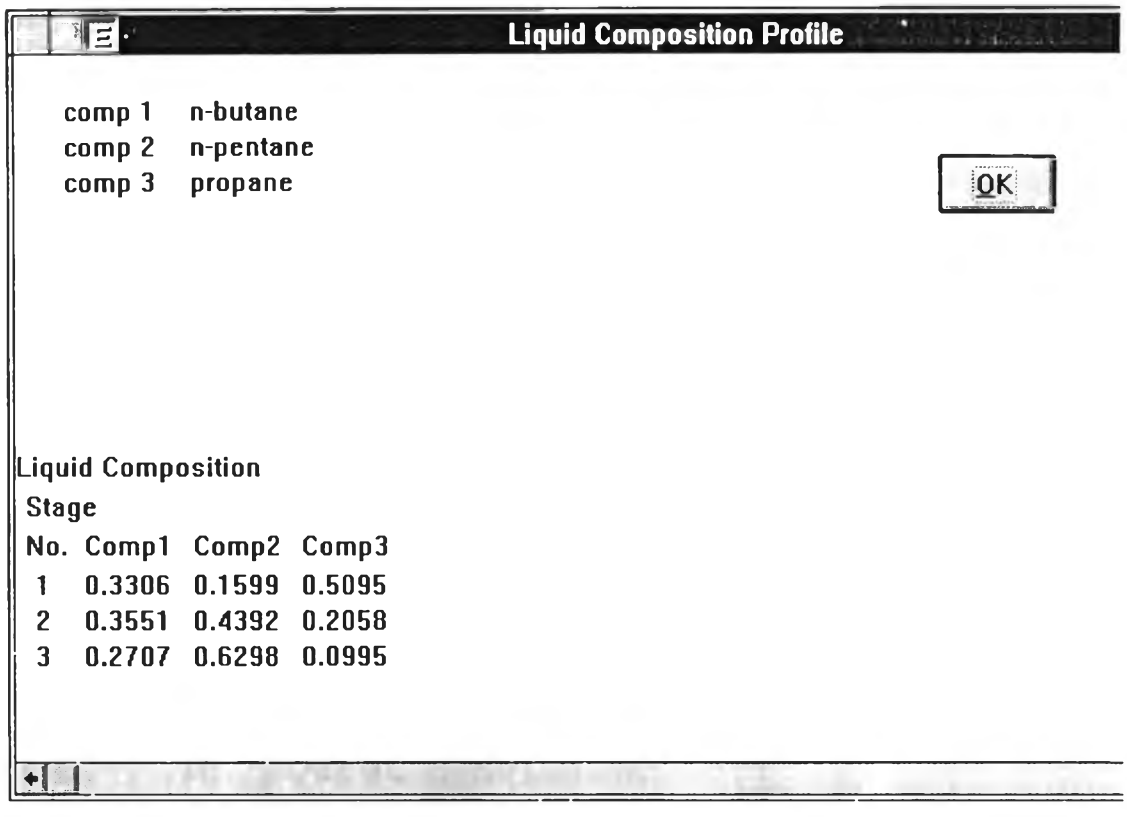

Figure 4.11 The liquid composition window.

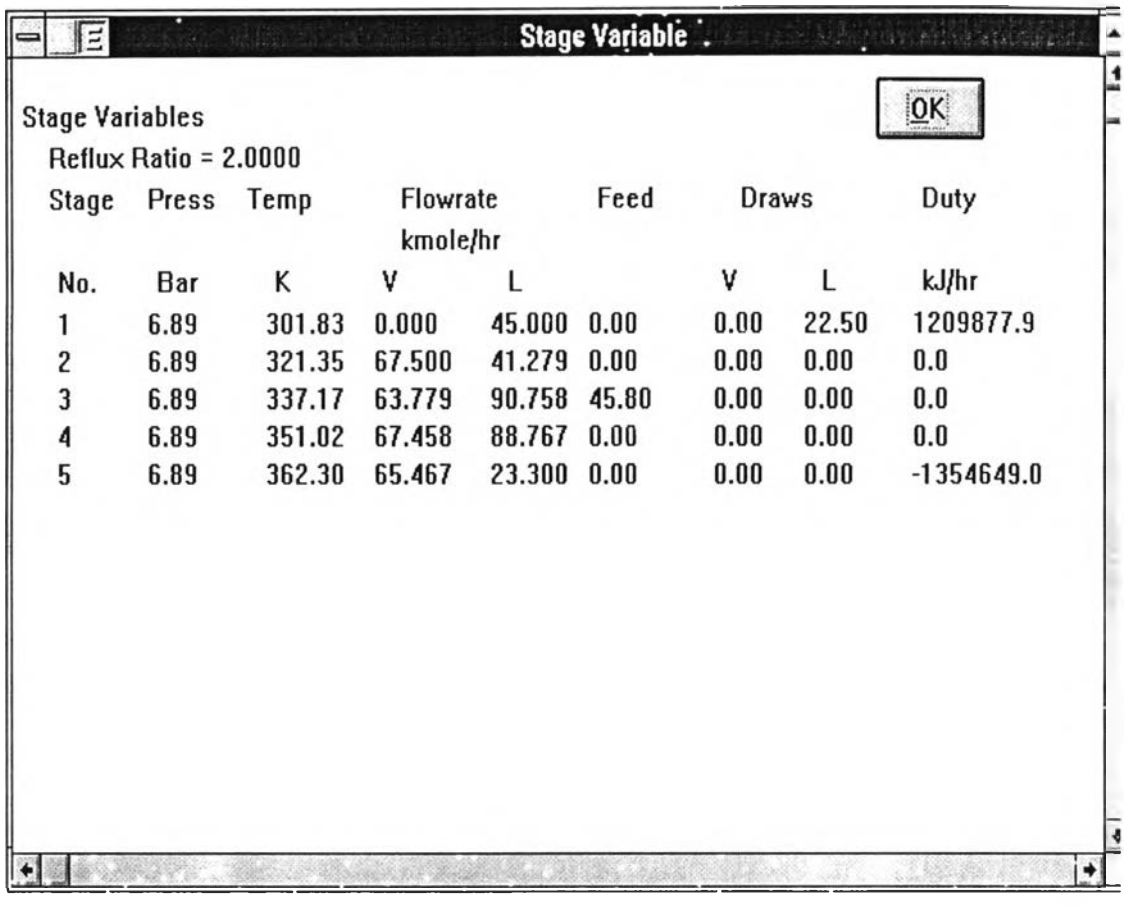

Figure 4.12 The stage variables window

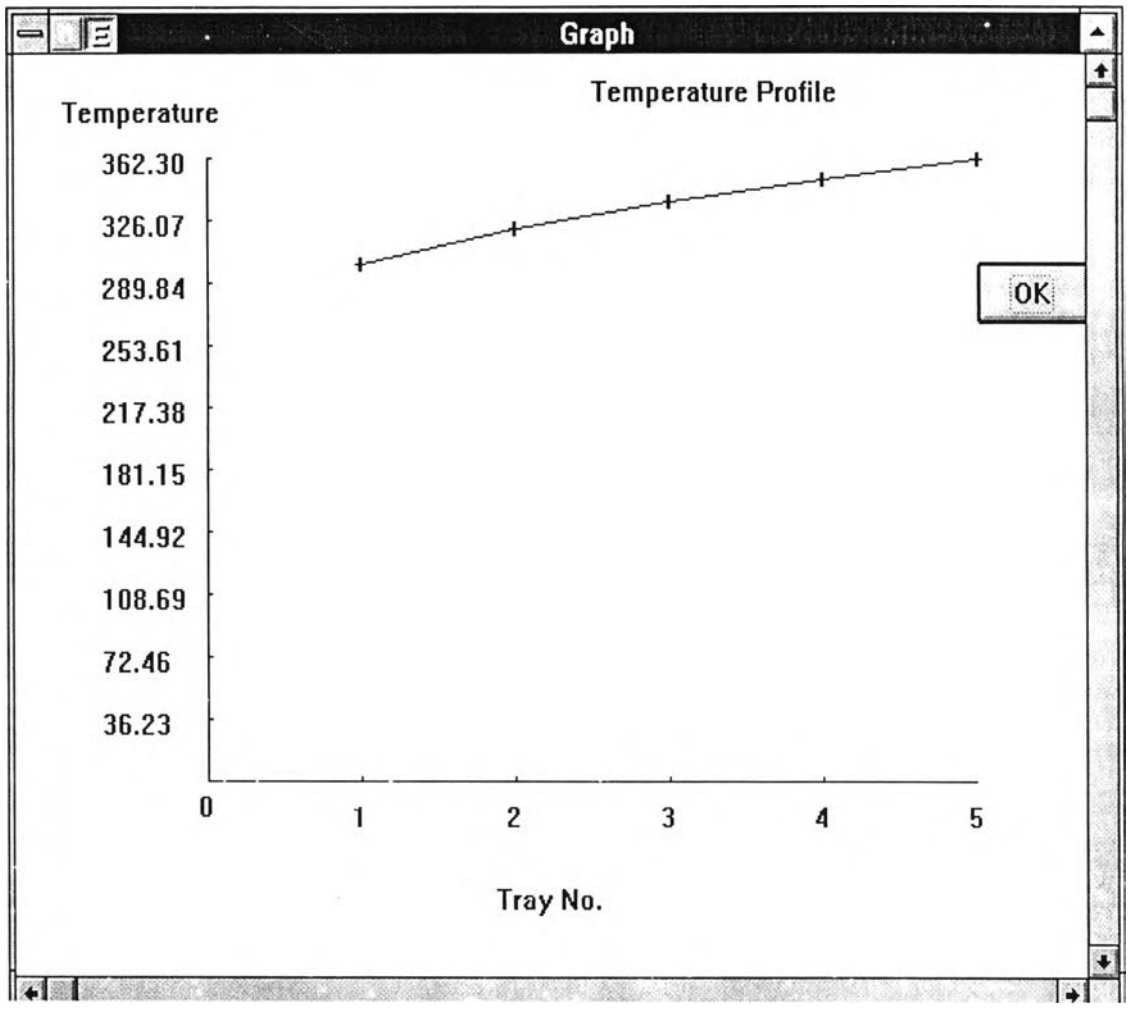

Figure 4.13 The temperature profile plotted on the output window.

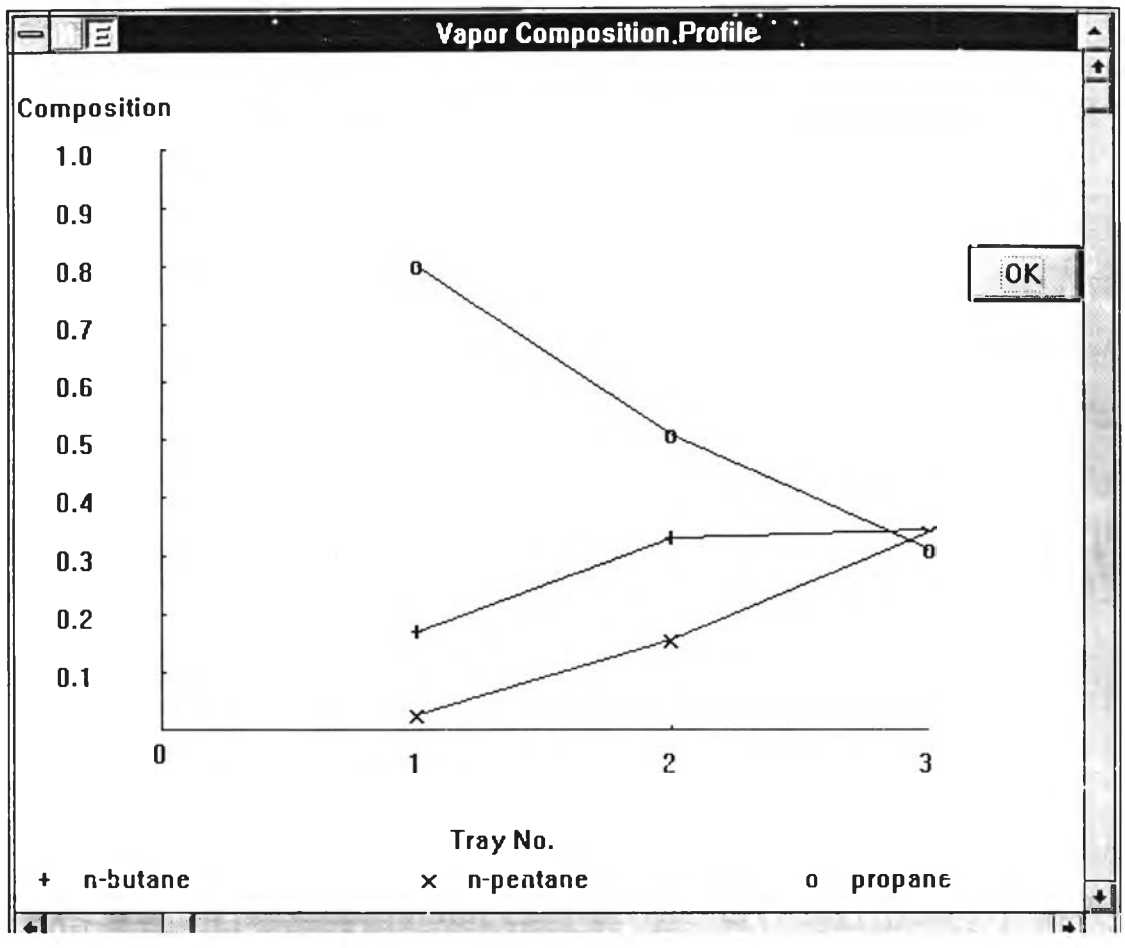

Figure 4.14 The vapor composition profile plotted on the output window.

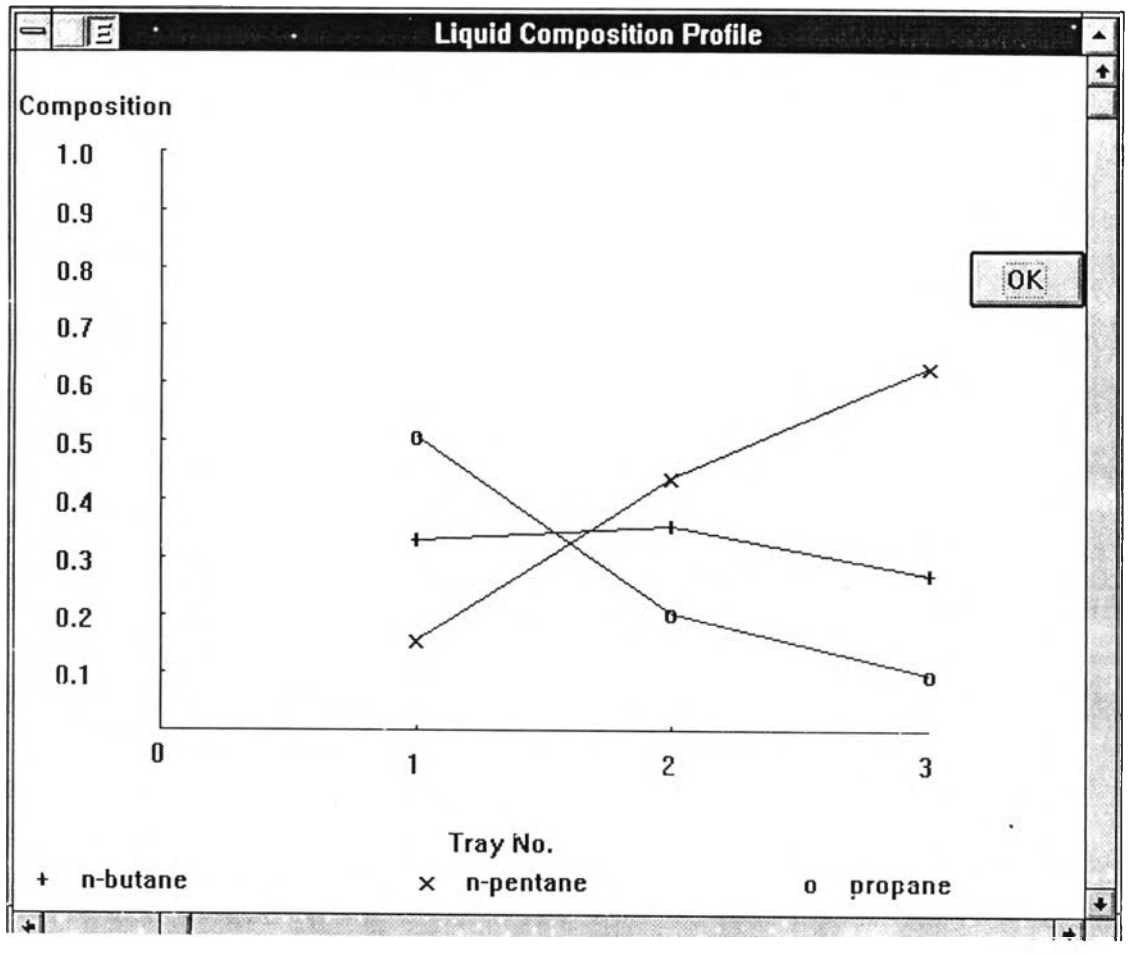

Figure 4.15 The liquid composition profile plotted on the output window.

ต้นฉบับ หน้าขาดหาย

Table 4.2 Summary of the output

Output	Details of Output
Check	To check Input Data
Product	Flowrate
- Top product	Composition
- Bottom product	Temperature
- Side stream	Pressure
All stages	Temperature distribution
	Composition distribution

4.2 The Details of Calculation Procedure

The data input window is used to declare variables for the calculating part. The calculation procedure is shown as follows:

1) All of variables have been defined as zero when the column configuration is specified by users. One of 2 dimensional array equals to the number of components and the other is the number of stages is the second dimension.

2) The input data is changed to the single or two dimensional arrays before calculating.

The single dimensional arrays are temperature (T), pressure (P), feed temperatures (T_f), feed pressures (P_f), feed flowrates (F), vapor (V) and liquid

(L) flowrates, vapor (W) and liquid (U) sidestreams and heat duties (Q). The indexes of those arrays are represented by numbers of equilibrium stage.

The two dimensional arrays are the phase equilibrium constant (K) and compositions of liquid, vapor and feed. Both indexes of the arrays are represented by numbers of components and equilibrium stages, respectively.

3) Variable initialization

The liquid bottom product from reboiler (L_N) is calculated from overall material balance that given in equation (3-6).

The pressure of each stage are defined by equation (4-1).

$$P_j = P_{j-1} + \frac{(P_N - P_1)}{N-1} \qquad (4\text{-}1)$$

where

P_N is pressure of reboiler (Bar).

P_1 is pressure of condenser (Bar).

The initial temperature of each stage is assumed to be linear from condenser to reboiler as shown in equation (4-2).

$$T_j = T_{j-1} + \frac{(T_N - T_1)}{N-1} \qquad (4\text{-}2)$$

where

T_N is temperature of reboiler (K).

T_1 is temperature of condenser (K).

The vapor interstage is defined from overall material balance of condenser.

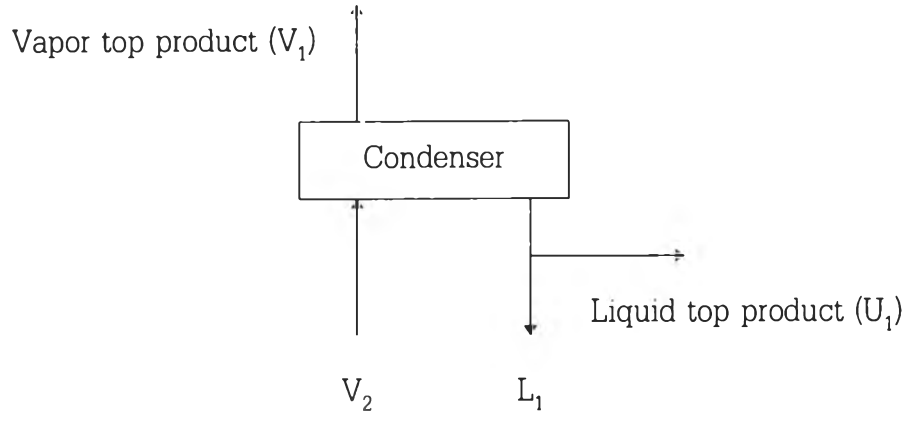

Figure 4.16 The model of the condenser (stage 1).

The model in figure 4.16 is assumed to be no vapor sidestream (W_1) and feed (F_1). Then the overall material balance is yielded as

$$V2 = V1 + U1 + L1 \qquad (4\text{-}3)$$

The equation (4-3) has two unknown, but we can find L_1 from reflux ratio. The reflux ratio is defined as the molar ratio of the liquid returning to stage 2 to the total flow of the liquid and vapor top product.

$$R = L_1/(U_1+V_1) \qquad (4\text{-}4)$$

or

$$L_1 = R^*(U_1+V_1) \qquad (4\text{-}5)$$

Substitute L_1 in equation (4-3) by (4-5) to find V_2.

$$V2 = V1 + U1 + R^*(U1+V1) \qquad (4\text{-}6)$$

This program initializes V_3 to V_N to be equal to V2.

4) The simulator firstly calculates from ideal condition to estimate the liquid composition in each stage as the initial guess.

5) Bubble temperature is calculated to find new T.

6) Temperature is rechecked by equation (3-30) and equation (3-31). Program terminates when the condition is true.

New V is determined from the method discussed in chapter III. Heat duties are calculated from equation (3-5) for the condenser and from equation (3-22) for the reboiler.

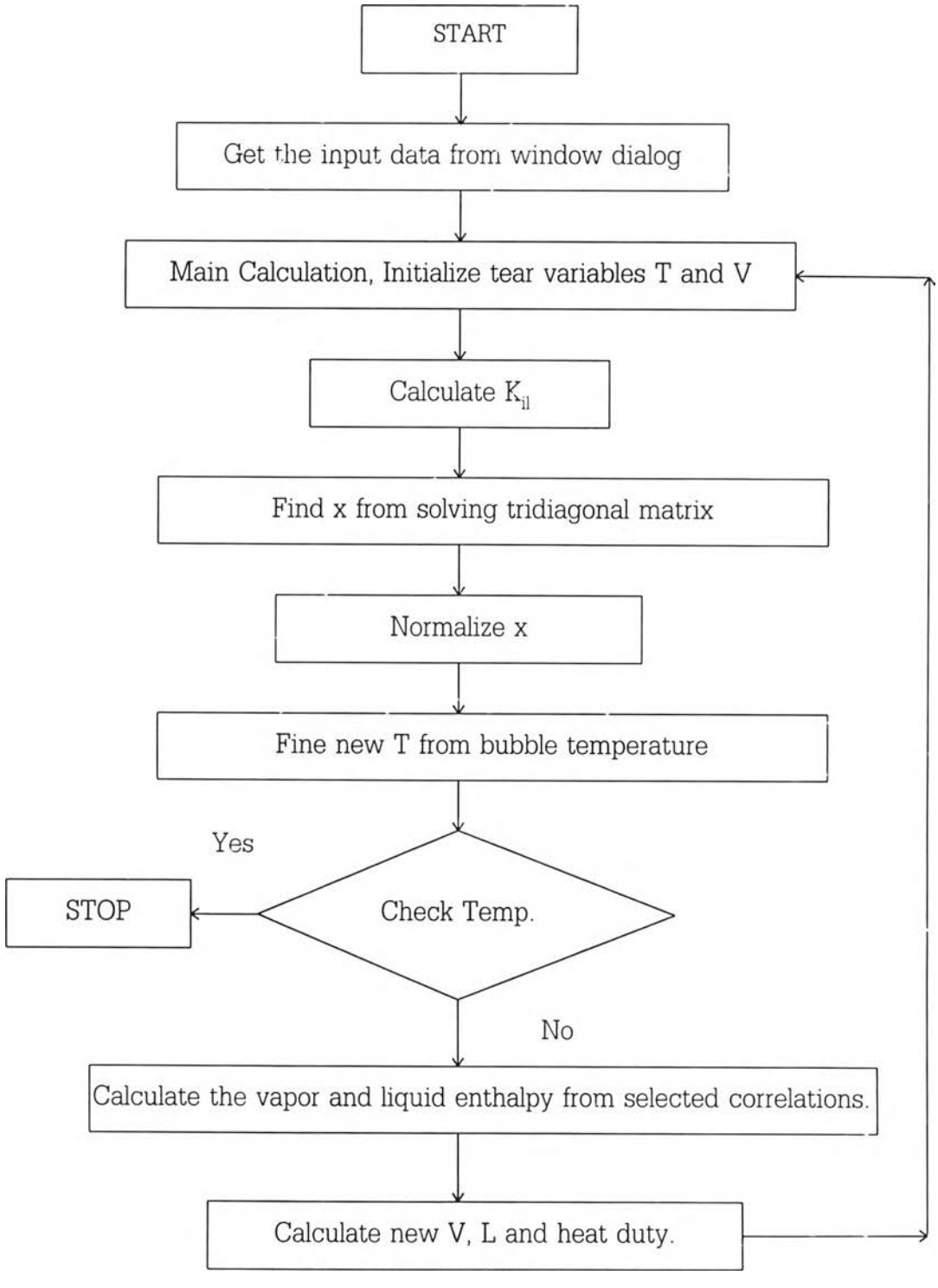

Figure 4.17 Flowchart of this simulator

4.3 An Overview of The Simulator

The distillation simulator displayed in this work is a Windows application consisting of the following main components:

- The frame window with the menu system, minimize icon, and maximize icon. The window has a title as "Distillation Column".
- The conventional distillation column shown on main window displays the input dialog of feed, top product, or bottom product when the left button is clicked at the active areas.

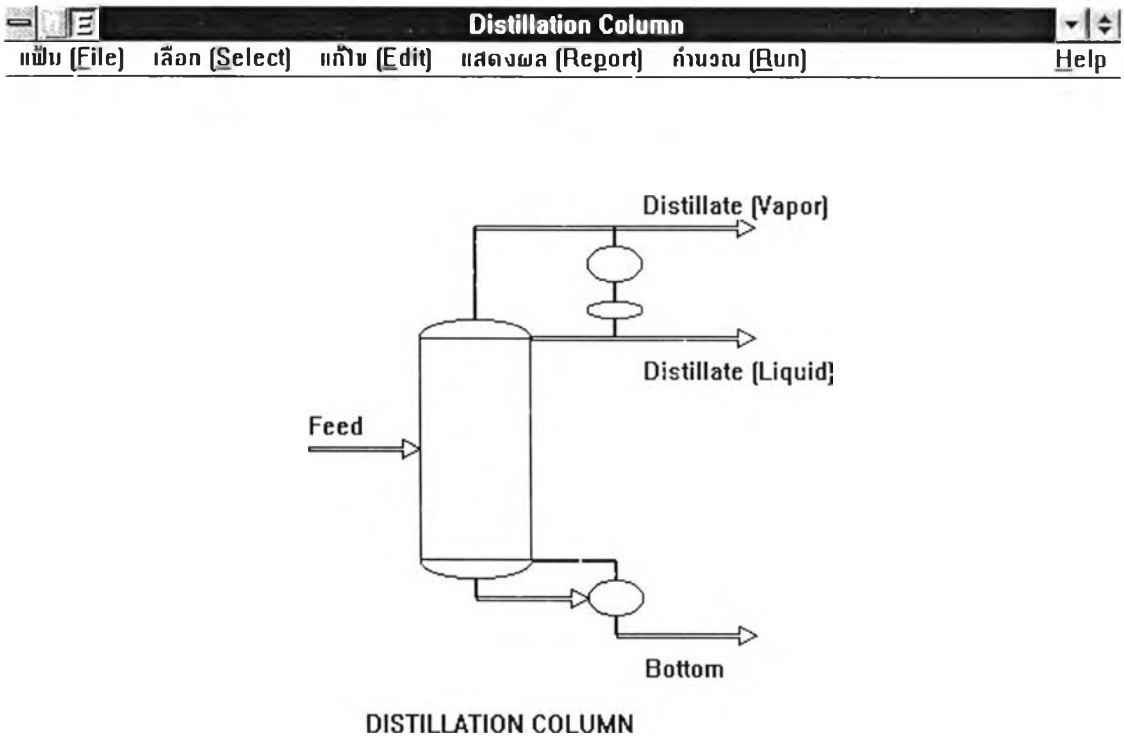

Figure 4.18 The main window of distillation simulator.

The Menu shown on the main window consists of many commands. The details for using each command is given as follows

4.3.1 The File Menu

The File menu consists of commands to start and to exit the application. The details of each command are shown in Table 4.3.

Table 4.3 Summary of the commands in the File menu.

Command	Function
New	To create a new the distillation case - show the column configuration dialog for enter the data. - show the window for select components.
Exit	To exit from the application.

4.3.2 The Selecting Menu

The Selecting menu provides commands for selection of components and methods for estimating the thermodynamic properties. The commands are shown in Table 4.4.

Table 4.4 Summary of commands in the Selecting menu.

Command	Function
Property Package...	To select a method to calculate the thermodynamic properties.
Ideal Case	Ideal case
SRK	Soave Redlich Kwong correlation
PR	Peng Robinson correlation
Components	Select components

4.3.3 The Edit Menu

The Edit menu provides commands to edit input data. Table 4.5 summarizes the commands in Edit menu.

Table 4.5 Summary of the commands in the Edit menu.

Command	Function
Feed	To input flowrate, conditions and location of feed streams.
Product	To input flowrate, temperature and pressure of product
Side stream	To input flowrate ad location of side streams
Energy Stream	To input heat transfer rate and location of streams (except the condenser and reboiler duty).
Column Configuration	Input Column Configurations, including • number of stages • number of feeds • number of side streams • number of energy streams • reflux ratio

4.3.4 The Report Menu

There are several commands for showing the input data and the results of calculation. Table 4.6 summarizes the commands in the Report menu.

Table 4.6 Summary of the commands in the Report menu.

Command	Function
Check	To show data that are input by user.
Input Data	- Column Configuration
	- Initial guess of product
	- Feed
	- Sidestreams
	- side exchanger
Result	To show the result of calculation.
Table	- Product
	- Vapor and liquid composition
Stage variables	To show temperature, pressure and flow in column
Graph	Temperature profile

4.3.5 The Run Menu

The Run command is used to run the program for solving distillation problems after all of necessary input data are defined.

4.3.6 The Help Menu

The Help file is very useful for users to start the simulator. The detail of help is following.

- How to use the simulator.
- Suggestion for input data.
- The column convention.
- The list of message from simulator.

The Help file of Distillation simulator is shown in figure 4.19.

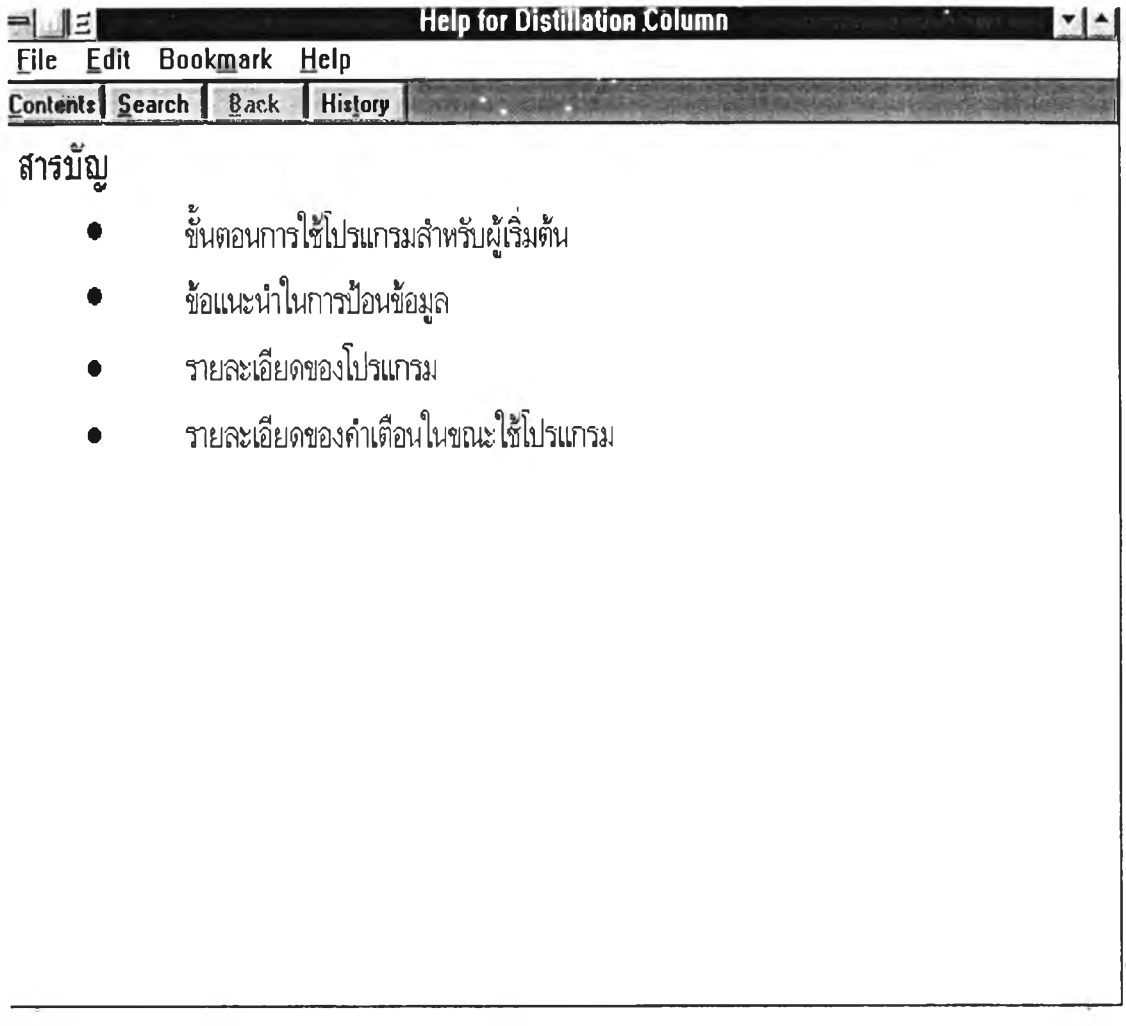

Figure 4.19 The Help file for distillation simulator.