

## **CHAPTER III**

### **DEVELOPMENT OF DYNAMIC SIMULATION SOFTWARE**

In Chapter II, the dynamic multicomponent stagewise calculation was introduced to determine the behaviour of column with full-order model. This approach allows prediction of compositions in distillation column when steady state is changed. However, in the same chapter the compartmental technique is also introduced to determine the behaviour of column with reduced-order model. To aid in both determinations, a dynamic simulation computer program has been developed in this chapter.

The following sections describe the development of the program, the features of the program and its limitations, the flowchart, and the procedure to run the program. Additionally, the detailed flowchart and the listing of the source program are presented in Appendix A and B, respectively.

#### **3.1 Development of program**

##### **3.1.1 Full-order Dynamic Simulation**

For a full-order model, Dynamic continuity equations of mass and energy for each tray are developed. The dynamic continuity equations state that the rate of accumulation of material (mass or energy) in a system is equal to the amount of

material entering and generated, less the amount leaving and consumed within the system :

$$\left[ \begin{array}{l} \text{rate of accumulation} \\ \text{of mass (energy)} \end{array} \right] = \left[ \begin{array}{l} \text{mass (energy) flow} \\ \text{into the system} \end{array} \right] - \left[ \begin{array}{l} \text{mass (energy) flow} \\ \text{out of the system} \end{array} \right] \\ + \left[ \begin{array}{l} \text{mass (energy) generated} \\ \text{within the system} \end{array} \right] - \left[ \begin{array}{l} \text{mass (energy) consumed} \\ \text{within the system} \end{array} \right]$$

The accumulation term is a first order time derivative of the total mass or energy. The flow terms are algebraic. This results in a first order ordinary differential equation that usually nonlinear. Material balances for each component and one energy balance is written. The component balances are modelled as equation (2-55) and an overall energy balance can be written as equation (2-56). The change in specific liquid enthalpy is usually very small compared to the total tray enthalpy. Therefore, the energy balance may be reduced to an algebraic relation that can be used to calculate the vapour rate leaving the stage. After that the Murphree vapour phase stage efficiency, equation (2-61), can be applied to find the actual vapour rate leaving the stage.

Following procedure can be used to solve the stage model. The procedure starts from the bottom and proceeds up through the column.

1. Calculate the equilibrium vapour composition and temperature from pressure and liquid composition by a bubble point calculation as presented by Figure 2.4 in chapter II.
2. Calculate the actual vapour composition from the Murphree vapour phase stage efficiency.
3. Calculated the vapour and liquid enthalpy from their composition and stage temperature.
4. Calculate the clear liquid density from composition and temperature.

5. Calculate the liquid rate leaving the stage from the Francis weir formula, equation (2-53).
6. Calculate the vapour flow leaving the stage from the energy balance.
7. Calculate the component and total mass derivatives.

### 3.1.2 Compartmental Dynamic Simulation

Development of a compartmental model follows similar steps of a full-order model but the dynamic continuity equations are different as shown in equation (2-77). Main assumption of the compartmental model is that the several trays can be grouped into a single compartment, therefore, a dynamic continuity equation can be grouped as a single stage. These mean the liquid and vapour leaving each compartment could be redefined. The equations describe the liquid and vapours leaving each compartment are shown by equations (2-78) through (2-81) for rectifying and stripping section respectively. The selection of compartment would be followed to guidelines of Benallou et al (1986) and Horton (1990) as reviewed in chapter II.

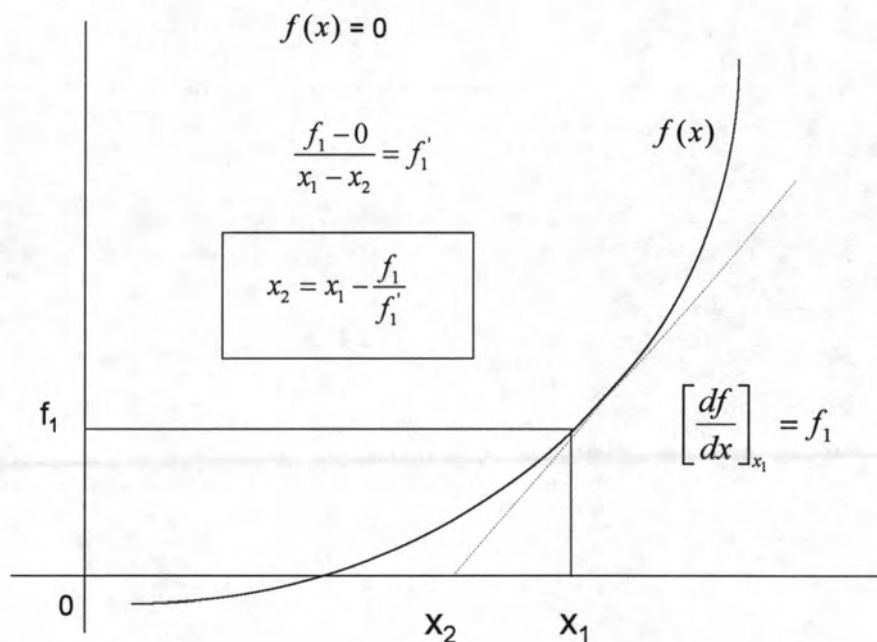
### 3.1.3 Numerical Methods

#### 3.1.3.1 Newton Raphson Method

Newton-Raphson is a powerful numerical method for thermodynamic calculations, such as the bubble point calculation. The analytical derivative is readily available for these calculations. Figure 3.1 presents the Newton-Raphson method graphically.

The method requires an initial estimate of the solution ( $x_1$ ). An analytical expression gives the derivative of the objective function at the estimate. The derivative is the tangent to the curve at this point. The next estimate ( $x_2$ ) is computed where the tangent intersects the  $x$  axis at  $f = 0$ . These convergence methods require

initial estimates for the solution. During the dynamic simulation, the solution at the previous time step is used for these estimates. This is very close to the solution at the current time step. The algebraic equations are solved very quickly, in only a few iterations.



**Figure 3.1 Newton-Raphson convergence.**

Source : William L. Luyben, Practical Distillation Control, Van Nostrand Reinhold, New York, pp. 38, 1992.

### 3.1.3.2 Euler Integration Method

The simplest possible numerical-integration scheme is Euler integration, illustrated graphically in Figure 3.2. Assume the ordinary differential equation is wished to solve.



$$\frac{dx}{dt} = f(x, t) \quad (3-1)$$

where  $f$  is, in general, a nonlinear function. It is needed to know where it is starting from; i.e., a known initial condition for  $x$  is needed.

$$x_{(0)} = x_0 \quad \text{at } t = 0 \quad (3-2)$$

Now if it is moved forward in time by a small step  $\Delta t$  to  $t = \Delta t$ , it can be got an estimate of the new value of  $x$  at  $t = \Delta t$ ,  $x_{(\Delta t)}$ , from a linear extrapolation using the initial time rate of change of  $x$ . The new value of  $x$  is approximately equal to the old value of  $x$  plus the product of the derivative of  $x$  times the step size.

$$x_{(\Delta t)} = x_{(0)} + \left( \frac{dx}{dt} \right)_{t=0} \Delta t \quad (3-3)$$

$$x_1 = x_0 + f_{(x_0, 0)} \Delta t \quad (3-4)$$

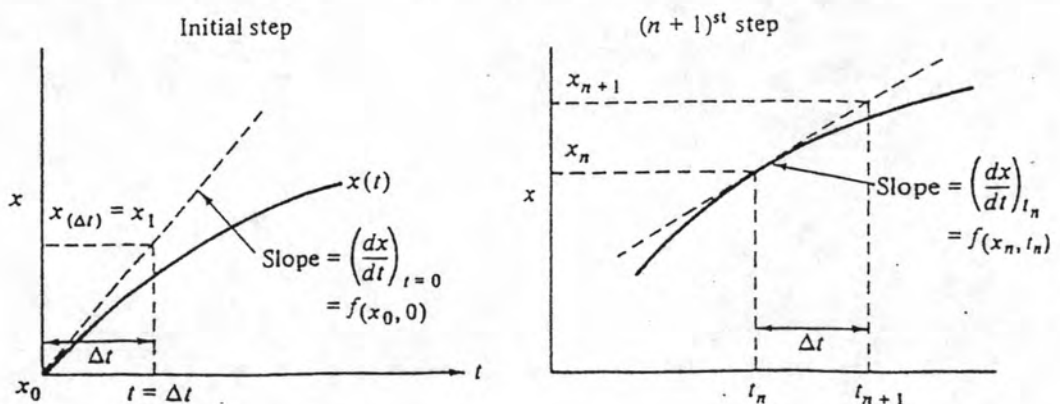


Figure 3.2 Graphical representation of Euler integration.

Source : William L. Luyben, Process Modeling, Simulation, and Control for Chemical Engineering, McGraw Hill Book Company, New York, pp. 132, 1981.

If the step size or integration interval is small enough, this estimate of  $x_{(\Delta t)} \equiv x_1$  will be very close to correct value. To step out in time another  $\Delta t$ , it can be estimated  $x_{(2\Delta t)} \equiv x_2$  from

$$x_{(2\Delta t)} = x_{(\Delta t)} + \left( \frac{dx}{dt} \right)_{t=\Delta t} \Delta t \quad (3-5)$$

$$x_2 = x_1 + f_{(x_1, \Delta t)} \Delta t \quad (3-6)$$

Generalizing to the  $(n+1)$ st step in time,

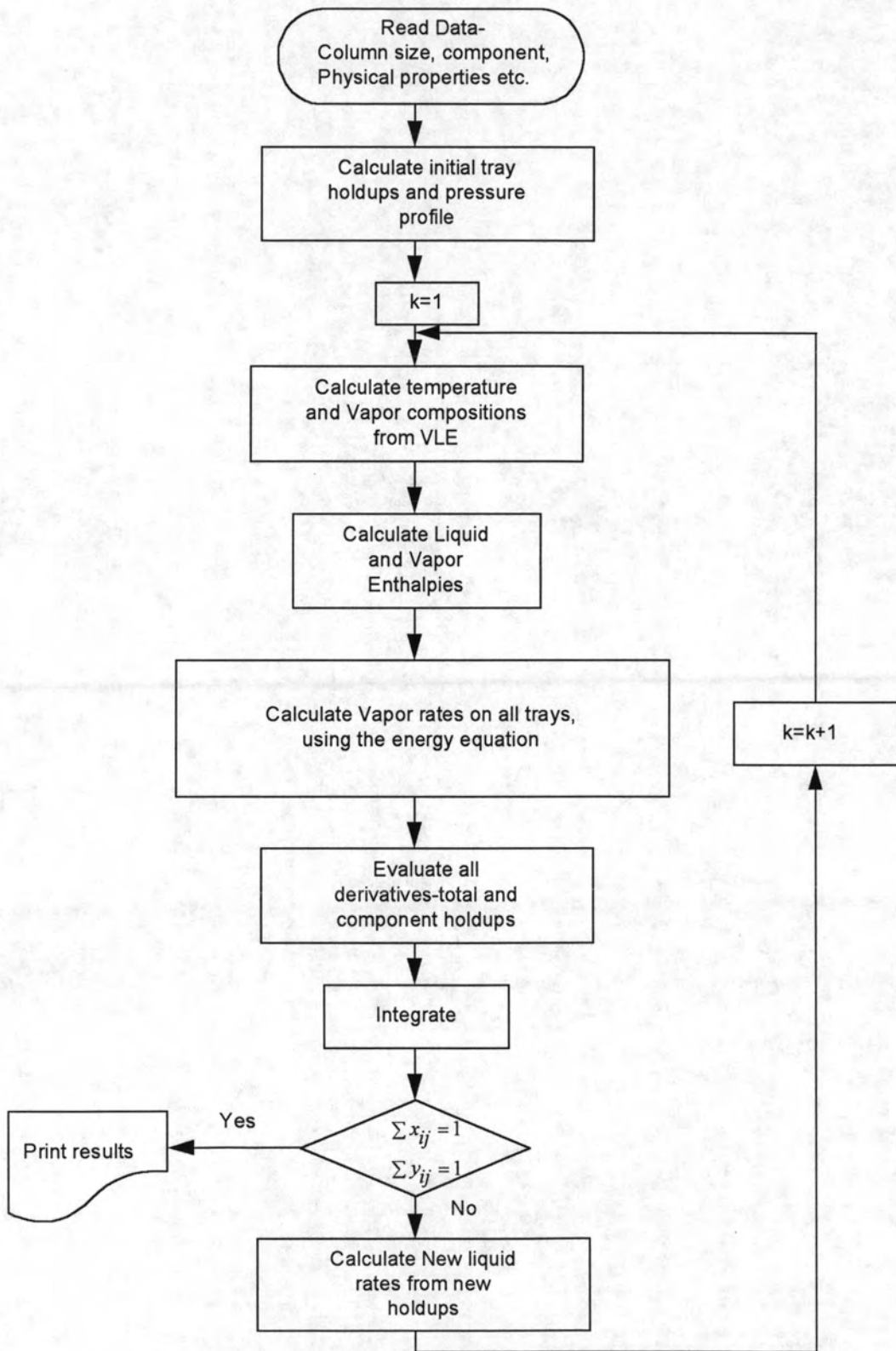
$$x_{n+1} = x_n + f_{(x_n, t_n)} \Delta t \quad (3-7)$$

Euler integration is clearly extremely simple to program.

### 3.2 Simplified Flowchart of Program

As shown in Appendix B, the simplified flowchart of program is presented by Figure 3.3. The program consists of the following sections :

1. Read data on the column size, components, feeds and initial conditions ( $T$ ,  $x$ , and  $L$ ).
2. Calculate initial tray holdups and the pressure profile.
3. Calculate temperatures and vapour compositions from the vapour-liquid equilibrium data, using subroutine BUBPT.
4. Calculate liquid and vapour enthalpies, using subroutine ENTH.
5. Calculate vapour rates on all trays, using the energy equation.
6. Evaluate all derivatives-total and component holdups.
7. Integrate.
8. Calculate new liquid rates from new holdups, using subroutine HYDRAU.
9. Go back to step 3 and repeat.



**Figure 3.3 Simplified Flowchart of Program**

### 3.3 Features and Limitations of Program

The present program was developed from an earlier version published in Process Modelling, Simulation, and Control for Chemical Engineers (1981) which programmed only for a full-order model. The program was coded in FORTRAN IV to utilize its powerful formatting features highly suitable to complex scientific, mathematical, engineering algorithms and it is executed on a personal computer. The flowchart notation used in Appendix A corresponded to specific program statements in Appendix B. The flowchart illustrated the algorithm used and the rudiments of programming in the 1977 version of the FORTRAN IV language.

The requirements needed to run the programs are :

Hardware : A personal computer with two disk drives and 640 K of random-access memory operating on the Disk Operating System (DOS command). To obtain a hard copy, a printer is recommended.

Software : A 3.5-inch double-sided, high-density, soft section diskettes containing the source and working program.

#### 3.3.1 Program Features

The source program was coded and edited using Program's Workbench software as line editor and identified by the filename of DYNAMICS.FOR (see Appendix B). The working program was compiled and ready-to execute version obtained with MICROSOFT FORTRAN Programming Software (Version 5.1). Its filename and extension were DYNAMICS.EXE. The capability of the present program is as follows :

- Determine thermodynamics properties of various components using S-R-K Equation of state.



– Determine the behaviour of multicomponent distillation column with full-order model.

– Determine the behaviour of multicomponent distillation column with reduced-order as compartmental model.

### 3.3.2 Program Limitations

– Maximum numbers of ten components and fifty stages are allowed.

– Pressure is assumed constant on each stage but varies linearly up the column from  $P_B$  in the base to  $P_D$  at the top.

– There is one feed plate onto which vapour feed and liquid feed is introduced.

– The reboiler, condenser and feed stage should be chosen as sensitive stages in their compartments but does not need to isolated in individual compartments.

## 3.4 Input Data and Procedure to Run the Program

### 3.4.1 Input Data Required

1. Number of components

2. Number of plates in the column (not including condenser and reboiler)

3. Number of trays in stripping section

4. Weir height in stripping and rectifying section

5. Weir length in stripping and rectifying section

6. Column diameter in stripping and rectifying section

7. Volumetric holdup in column base and reflux drum

8. Characteristic of compartment (not including condenser and reboiler)

9. Pressure in top and bottom of column
10. Reboiler heat duty
11. Reflux rate and vapour product from reflux drum
12. Murphree vapour-phase tray efficiency
13. Feed data, i.e., Liquid and vapour feed flowrate, Liquid and vapour temperature, and Liquid and vapour feed composition
14. Initial conditions for all stages.

Note that the program accepts British Engineering Unit only.

#### 3.4.2 Procedure to run the Program

##### Step 1 : Start-up Procedure

Switch on the personal computer and boot the system with DOS commands. Load the working program from file DYNAMICS.EXE.

##### Step 2 : Input Stream Data

The program will prompt the user to input all necessary data by selection number from main menu on the display screen as shown in Figure 3.4. Caution : The name of component must be typed in CAPITAL LETTER.

##### Step 3 : Output of Results

The results of simulation will be written into a data file namely RESULT.DAT and will be displayed consecutively: table of liquid compositions for each stage in various times. In case a hard copy (printout) is desired, use the editor programming to open a data file and print it by editor's printing command.

\*\*\*\* MAIN MENU \*\*\*\*

- 0) Exit to Dos
- 1) Components Database
- 2) Characteristic of Column
- 3) Operating Conditions
- 4) Feed Data
- 5) Initial Conditions
- 6) Edit Input Data
- 7) Save Input data
- 8) Run
- 9) Reporting & Reviewing the results

Please ENTER your selection : \_\_\_\_

**Figure 3.4 Main menu of Program**