CHAPTER 4
NUMERICAL METHOD AND SIMULATION EXAMPLE

4.1 Introduction

Digital simulation is a powerful tool for solving the equations describing chemical engineering systems. However, digital simulation is not completely without its problems. The principal difficulty arises in integration. This must be done numerically on a digital computer since the digital machine is not a continuous device but merely a very fast desk calculator. Numerical integration involves approximating continuous differential equations with discrete finite-difference equations. This chapter will begin discussion of digital simulation by developing some of the more important and useful numerical methods. Then the example of application of these methods to a distillation column will be studied.

4.2 Numerical Method

The numerical method is used to solve these models. There is no one method that works best for all models. The appropriate method will improve the speed of the simulation at each time step. For this thesis ,there are two methods used :

4.2.1 Euler method

The simplest possible numerical-integration scheme (and the most useful) is Euler. The following simple first order Euler integrator will be used to integrate the model:

$$x_{n+1} = x_n + (\frac{dx}{dt})_n \Delta t \qquad (4.1)$$

(Initial condition: at $t=0$ $\quad x = x_0$)

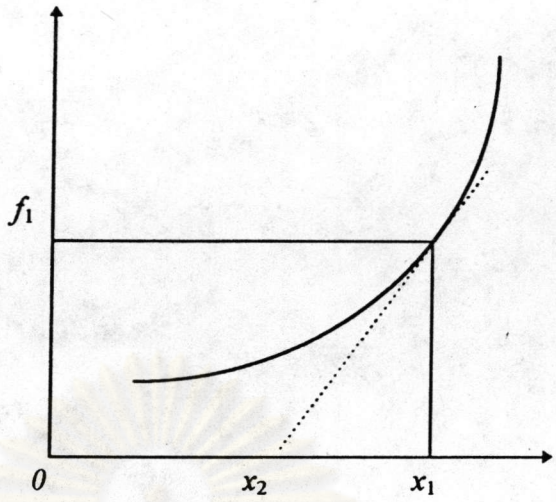
where x is the function of time (t). This numerical-integration method is for solving the ordinary differential equations. The Euler integrator is very easy to implement and is very effective at solving a system of nonstiff differential equations. The Euler integrator works well for solving the distillation model that developed in this thesis. If the step size (the integration interval) is small enough, this estimate of x will be very close to the correct value.

Models that include vapor hydraulics and pressure dynamics are stiff. It is usually more efficient to use an implicit integrator such as LSODE for such stiff systems. It is important to remember the difficulty with stiffness is that it slows down the simulation. Because the computational speed of computers has dramatically increased over a short period, systems that were considered a few years ago to be too stiff to solve explicitly are now quickly solved by present day computers. Explicit methods are generally easier to implement than implicit integrators and the solution behavior of an explicit integrator is easier to follow than an implicit integrator. This is a big benefit when you are debugging your simulation. Example assume an equation of system is $dx/dt = L - V + B$ and at $t=0$ $x = x_0$. Now if move forward in time by a small step Δt to $t=t_1$

$$x_1 = x_0 + (\frac{dx}{dt})_{t=0} \Delta t \tag{4.2}$$

4.2.2 Newton-Raphson method

The conventional simulation of a distillation column requires solving algebraic equations before integrating the system of ordinary differential equations. This iterative convergence method that is very useful for distillation problem is the Newton-Raphson method. The Newton-Raphson method requires the objective function to be written in the form $f(x)=0$. This method requires the first derivative of the function to be evaluated, preferably analytically. Newton-Raphson is a very powerful numerical method for thermodynamic calculation, such as the equilibrium bubble point. The analytical derivative is readily available for these calculations. Figure 4.1 presents the Newton-Raphson method graphically.



$$\frac{df_1}{dt} = \frac{f_1 - 0}{x_1 - x_2}$$

$$x_2 = x_1 - \frac{f_1}{(\frac{df_1}{dt})}$$

Fig.4.1 Newton-Raphson convergence.

The Newton-Raphson 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 $f=0$. This solution procedure is very similar to the Wegstein method but a tangent is used to compute the next estimate instead of a secant.

4.3 Procedure of Simulation

4.3.1 Distillation column of this thesis

The distillation column of the thesis is shown as figure 4.2.

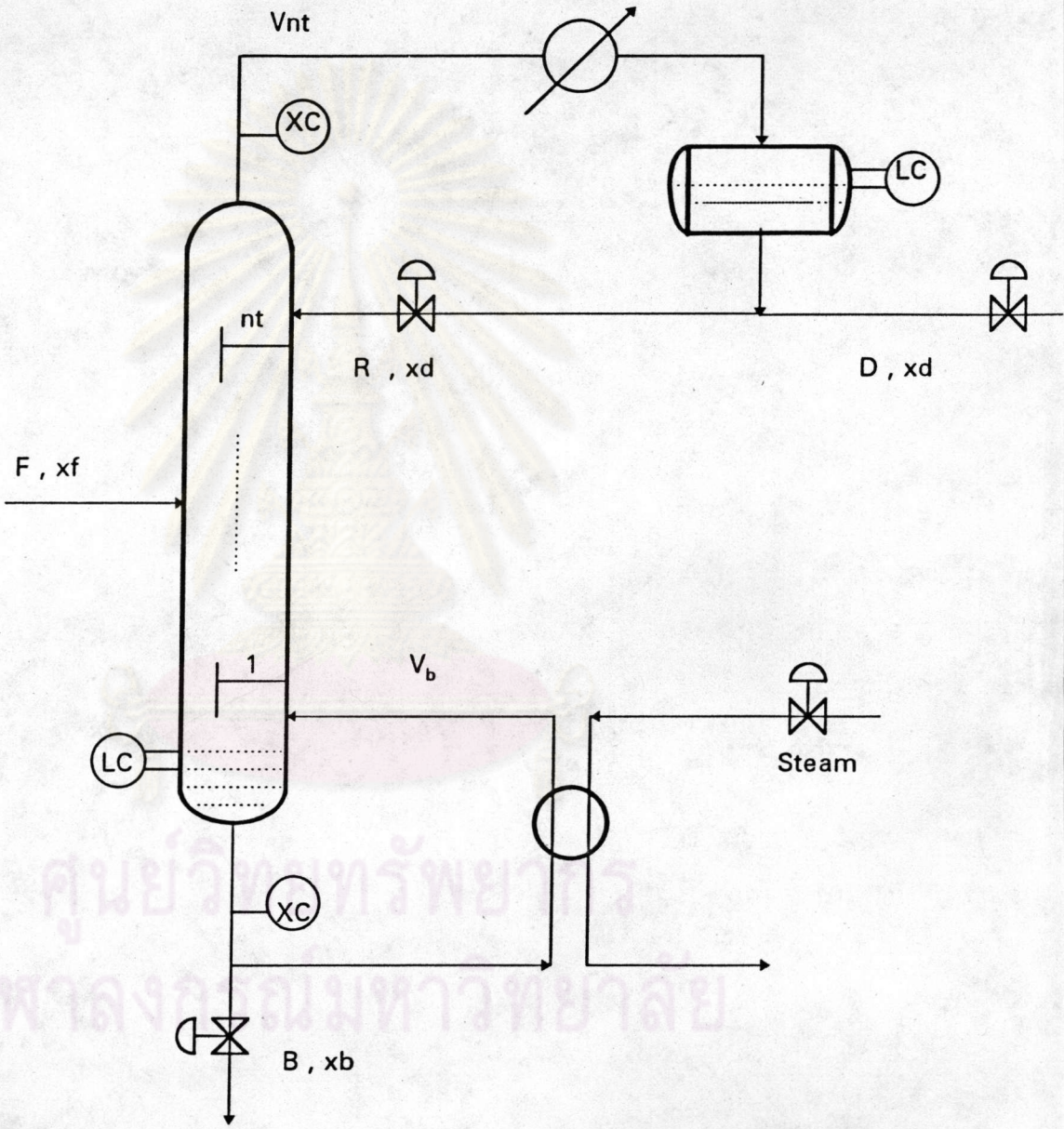


Fig.4.2 Distillation column

4.3.2 Flow diagram of simulation

The procedure to write a conventional simulation are followings.

1. Create a data file with the tower mechanical, instrument, and physical propertydata,i.e, column diameter (D), weir lenght (W_{len}) ,etc.
2. Specify the initial conditions of the state variables. If the program has been made the previous runs,a snapshot of the process variables is saved in a data file that can be used as the initial conditions. If this is the first run, specify a set consistent initial conditions.
3. Calculate the right hand side terms of each equation,i.e, enthalpy (H), mole fraction (y) ,etc.
4. Calculate the derivatives of each stage starting with the bottom sump and working up to the column.
5. Calculate the derivatives for the condenser and reflux accumulator .
   Integrate all the derivatives.
6. Calculate the terms for controllers.
7. Increment time by the integration time step.
8. Go back to step 3 and continue.

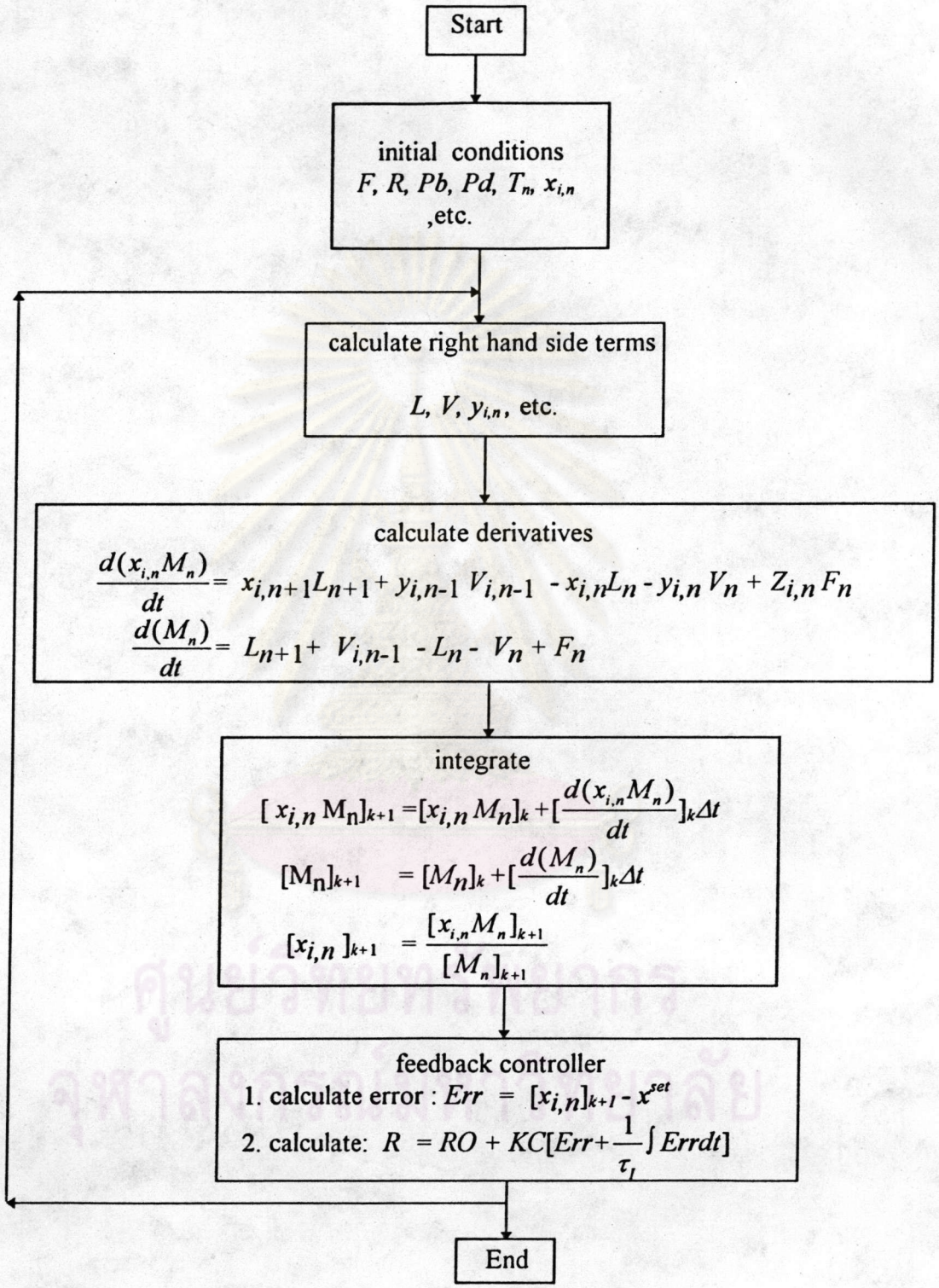


Fig.4.3 Flow diagram of simulation

4.3.3 Equilibrrium Bubble Point Calculation

The development of an equilibrium stage model requires the calculation of the vapor composition and temperature in equilibrium witha known pressure. This is a bubble point calculation. Equation (5.3) will be used for thermodynamic model. A starting temperature is guessed. The Reidel's equation is used to compute the vapor pressure. A single dimensional Newton-Raphson method is used to converge temperature and compute the equilibrium vapor composition. The relations and a graphical representation of the solution are presented :

$$y_i = \frac{\gamma_i x_i P_i^*}{P} \tag{4.3}$$

$$P^*_i = P \exp(A_i - \frac{B_i}{T_r} + C_i ln(T_r) + D_i T_r^6) \tag{4.4}$$

$$f = 1 - \Sigma y_i = 0 \tag{4.5}$$

$$\frac{df}{dT} = \frac{y_i[\frac{B_i}{T_r^2} + \frac{C_i}{T_r} + 6D_i T_r^5]}{T_r} \tag{4.6}$$

converge T: $$T_{k+1} = T_k + \frac{f}{(\frac{df}{dT})} \tag{4.7}$$