

CHAPTER V

PROGRAM DEVELOPMENT AND SIMULATION OF AN EXISTING DEBUTANIZER COLUMN

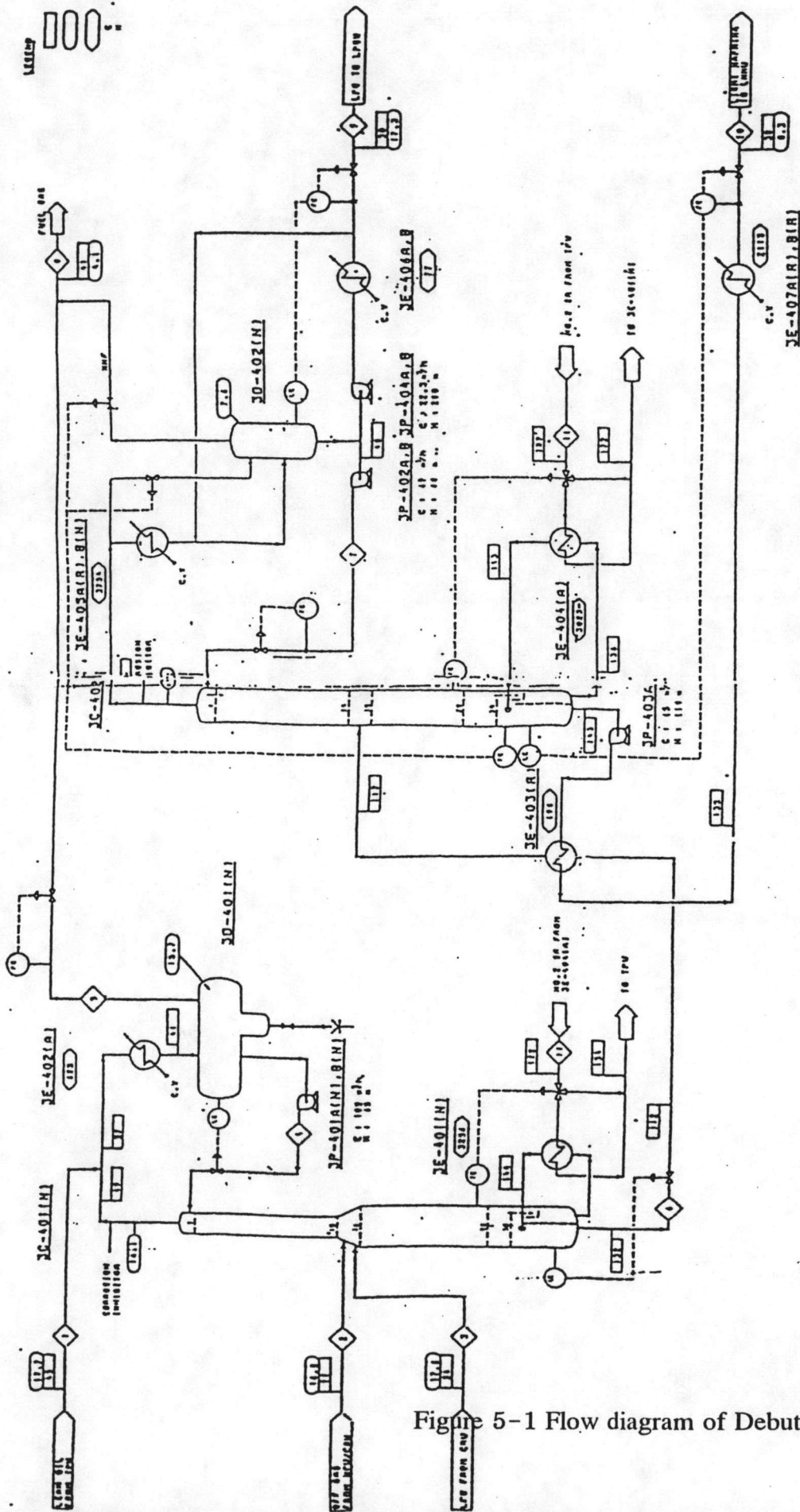
5.1 Basic process for Debutanizer column

Debutanizer column is one of two column in Gas recovery Unit. In this unit, The LPG and the Light naphtha are recovered from the lean oil from the Topping unit, the combined off gas from the NPU/CRU and the raw LPG from the CRU. This unit consists of two columns, one is the deethanizer where the off gas company of such as H_2 , C_1 and C_2 is stripped and the other is the debutanizer where the LPG and the Light naphtha are separated the former column is a fractional absorber and the latter column is a fractionation.

Debutanizer column employs a reboiler at the bottom of the column to generate its own stripping vapor, which strip the constituents to be excluded from the bottom product, and employ a condenser at the top of the column to provide reflux, which removes the constituents to be excluded from the overhead products. In the column, the vapor rises through the column, contacting the down flowing reflux stream, as a result, the lighter materials concentrate at the top of the column, the heavier materials at the bottom.

5.2 Program development for dynamic simulation

The configuration of an existing debutanizer column from which the plant-operating conditions is shown in Fig.5-1). The topper has a condenser and reflux accumulator. The bottom has a reboiler. The product LPG



Stream No.	Flow Rate		Pressure		Temperature		Composition		Control		Instrumentation	
	kg/hr	m ³ /hr	kg/cm ²	psia	°C	°F	wt%	mol%	Valve	Control	Symbol	Location
1	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
2	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
3	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
4	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
5	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
6	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
7	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
8	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
9	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100
10	100	0.000	2.0	29.4	25	77	95	5	100	0	1	100

Figure 5-1 Flow diagram of Debutanizer column

come out the condenser and the LN come out the column bottom. The column consists of twenty-five plates. Other column specifications are noted in the figure.

As for the simulation, the stages are numbered upward, starting from the bottom column through the top of column.

The general model was developed in chapter 4. The specific column simulated is assumed to have the following equipment configurations and conditions:

1. There is one feed plate onto which vapor feed and liquid feed are introduced.
2. Pressure is constant and known on each tray. It varies linearly up the column from P_B in the base to P_D at the top.
3. Coolant and steam dynamic are negligible in the condenser and reboiler.
4. Vapor and liquid products D_V and D_L are taken off the reflux drum and are in equilibrium. Dynamics of the vapor space in the reflux drum and throughout the column are negligible.
5. Liquid hydraulics are calculated from the Francis weir formular.
6. Volumetric liquid holdups in the reflux drum and column base and held perfectly constant by changing the flow rate of bottoms product B and liquid distillate product D_L .
7. Dynamic changes in internal energies on the trays are much faster than the composition or total holdup changes, so the energy equation on each tray is just algebraic.
8. Reflux R and heat input to the reboiler Q_R are the manipulated variables. In this program, they are simply held constant, thus giving the openloop response of the column.

The program of this dynamic simulation model has the following steps:

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

Note that the program accepts British Engineering Unit only.

2. Calculate initial holdup of all trays.

At the column base, molar liquid holdup (MB) is calculated from volumetric holdup in column base (MVB) :

$$MB = \frac{MVB \times \rho}{MWA} \quad 5-1)$$

When $MWA =$ molecular weight average

At $N=1$ to NF tray, molar liquid holdup ($M(N)$) is calculated from liquid flowrate (LO) and volumetric liquid holdup on trays (MV) by using Francis weir formula:

$$LV(N) = \frac{LO(N) \times MWA}{\rho} \quad 5-2)$$

$$MV(N) = \left[\left(\frac{LV(N)}{999WLS} \right)^{66667} + \frac{WHS}{12} \right] \frac{(3.1416)(DS)^2}{4(144)} \quad 5-3)$$

$$M(N) = \frac{MV(N) \times \rho}{MWA} \quad 5-4)$$

At $N = NF + 1$ TO NT tray, molar liquid holdup ($M(N)$) is calculated from liquid flowrate (LO) and volumetric liquid holdup on tray (MV) by using Francis weir formula:

$$LV(N) = \frac{LO(N) \times MWA}{\rho} \quad 5-5)$$

$$MV(N) = \left[\left(\frac{LV(N)}{999WLR} \right)^{66667} + \frac{WHR}{12} \right] \frac{(3.1416)(DR)^2}{4(144)} \quad 5-6)$$

$$M(N) = \frac{MV(N) \times \rho}{MWA} \quad 5-7)$$

3. Calculate pressure profile of all tray from top pressure (PD) and bottom pressure (PB)

At $N=1$ to NT :

$$P(N) = \frac{PB - (N(PB - PD))}{NT} \quad 5-8)$$

4. Calculate the temperature and vapor composition from vapor and liquid equilibrium data.

Calculation of VLE from an equation of state is based on the equilibrium equations

$$Y_i \hat{\phi}_i^v = X_i \hat{\phi}_i^L \quad 5-9)$$

Application of equation 5-9) requires the availability of a single PVT equation of state suitable for both liquid and vapor mixtures. Such an equation is invariably explicit in pressure, and thus expressions for the $\hat{\phi}_i$ are computed from GRK, SRK, and PR equation of state in the following:

For GRK equation of state, from equation 4-12)

$$\ln \phi_i = (Z-1) \frac{B_i}{B} - \ln(Z - BP) - \frac{A^2}{B} \left(2 \frac{A_i}{A} - \frac{B_i}{B} \right) \ln \left(1 + \frac{BP}{Z} \right)$$

For SRK equation of state, from equation 4-17)

$$\ln \phi_i = \frac{b_i}{b} \left(\frac{PV}{RT} - 1 \right) - \ln \left(\frac{PV}{RT} - B \right) - \frac{A}{B} \left(2 \frac{a_i^{0.5}}{a^{0.5}} - \frac{b_i}{b} \right) \ln \left(1 + B \frac{RT}{PV} \right)$$

For PR equation of state, from equation 4-23)

$$\ln \phi_i = \frac{b_i}{b} (Z-1) - \ln(Z-B) - \frac{A}{2\sqrt{2}B} \left(\frac{2 \sum_{k=1}^N x_k a_{ki}}{a} - \frac{b_i}{b} \right) \left(\frac{Z+2.414B}{Z-0.414B} \right)$$

The resulting expressions for the $\hat{\phi}_i$ are generally complicated, and the calculations involve considerable iteration. A schematic block for a calculation is shown in Fig. 5-2). One starts with given values of P and the X_i , and with the physical properties necessary for evaluation of all parameters appearing in the equation of state. The temperature and the vapor composition are unknowns and are to be calculated. However, the $\hat{\phi}_i^L$ depend on P , and the $\hat{\phi}_i^v$ depend on P and the Y_i . We therefore include as input initial estimates for T and for the Y_i . The first step in the solution is calculation of the $\hat{\phi}_i^L$ and $\hat{\phi}_i^v$ from equation 4-12), 4-17) and 4-23). Given these initial estimates of the $\hat{\phi}_i$, one can compute a set of equilibrium K - values:

$$K_i = \frac{\phi_i^L}{\phi_i^v} \quad 5-10)$$



Equation 5-10) is merely a rearrangement of equation 5-9), incorporating the definition $K_i = Y_i/X_i$. New estimates of the Y_i then follow immediately from equation 5-11)

$$Y_i = K_i X_i \quad (i=1, 2, \dots, N) \quad 5-11)$$

Each y_i is determined from Eq. (5-9) by an independent calculation; the condition $\sum y_i = 1$ has nowhere been imposed. Ultimately, the results must satisfy this condition, but it is unlikely that first estimates of the y_i from Eq. (5-9) will conform to it. In any event $\sum y_i$ is a key quantity in this scheme, and our next step is to sum the calculated y_i 's.

A set of y_i 's is now available from which we can recalculate the $\hat{\phi}_i^v$ by Eq. (4-12, 17, 23) for the first iteration we make this calculation immediately. However, the calculated y_i 's are first normalized, each value being divided by $\sum y_i = \sum (K_i x_i)$. This ensures that the set of y_i 's used for the calculation of the $\hat{\phi}_i^v$ do sum to unity. Once the $\hat{\phi}_i^v$ are determined, the inner loop of the block diagram is completed by a recalculation of the y_i 's; since T , P , and the x_i are the same as for the preceding calculation, the $\hat{\phi}_i^v$ remain unchanged.

Again we calculate $\sum y_i$; since this is a second iteration. The new $\sum y_i$ is compared with the sum found in the first iteration. If it has changed, the $\hat{\phi}_i^v$ is recomputed and another iteration starts. This process is repeated until the change in $\sum y_i$ from one iteration to the next is less than some preset tolerance. When this condition is realized, the next step is to ask whether $\sum y_i$ is unity. If it is, the calculations are complete; the computed values of the y_i are those of the equilibrium vapor phase, and the pressure assumed initially is the equilibrium pressure.

If $\sum y_i \neq 1$, then the assumed value of T must be adjusted according to some reasonable scheme. If $\sum y_i > 1$, the assumed pressure is too low; if $\sum y_i < 1$, it is too high. The entire iterative procedure is reinitiated with a new temperature. In the first iteration, normalized values of the last calculated set of y_i 's may be used for computation of an initial set of the $\hat{\phi}_i^v$.

The scheme just outlined, although rational and straightforward in principle, can be difficult to implement in practice. Depending upon the system, the conditions, and the equation of state, convergence problems may be encountered, and it is sometimes essential to have available at the outset very sharp estimates of the equilibrium T and y_i 's.

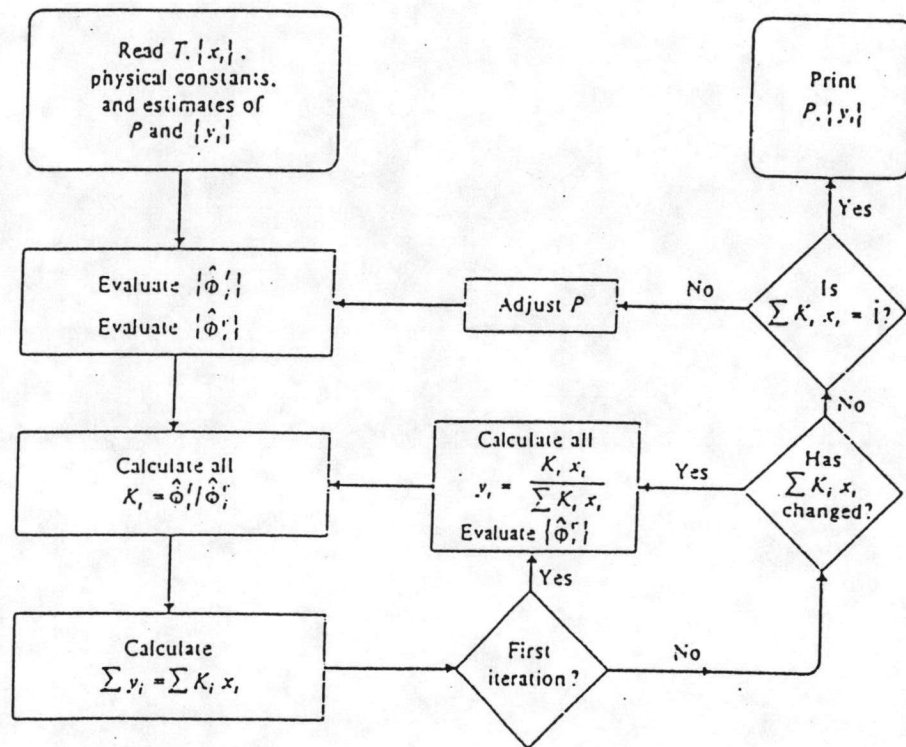


Figure 5-2 A Schematic Block for calculation of VLE

Source : Hendric C. Van Nees and Michael M. Abbott, Classical Thermodynamics of Nonelectrolyte Solutions, pp 284, Mc Graw-Hill Book Company, USA, 1984

5. Calculate liquid and vapor enthalpies, using GRK, SRK and PR equation of state :

$$\Delta H' = RT^2 \int_0^p \left(\frac{\partial Z}{\partial P} \right)_T \frac{dp}{\rho} - RT(Z-1)$$

For GRK equation of state, from equation 4-32)

$$\frac{H-H^*}{RT} = Z-1-1.5\frac{A^2}{B} \ln\left(1+\frac{BP}{Z}\right)$$

This equation can be used with both liquid and vapor phase.

For liquid phase,

$$\frac{HL-H^*}{RT} = Z-1-1.5\frac{AL^2}{BL} \ln\left(1+\frac{BL*P}{ZL}\right) \quad 5-12)$$

$$HL^* = \sum_i X_i H_i^*$$

$$AL = \sum_i X_i A_i$$

$$BL = \sum_i X_i B_i$$

For vapor phase,

$$\frac{HV-H^*}{RT} = ZV-1-1.5\frac{AV^2}{BV} \ln\left(1+\frac{BV*P}{ZV}\right) \quad 5-13)$$

$$HV^* = \sum_i Y_i H_i^*$$

$$AV = \sum_i Y_i A_i$$

$$BV = \sum_i Y_i B_i$$

ZB and ZV is calculated from cubic equation by using Newton Raphson method,

SRK equation of state, from equation 4-33)

$$\frac{H - H^*}{RT} = Z - 1 - \frac{A}{B} \left[1 - \frac{T}{a} \left(\frac{da}{dT} \right) \right] \ln \left(1 + \frac{B}{Z} \right)$$

$$T \left(\frac{da}{dT} \right) = \sum_i \sum_j x_i x_j m_j (a_i a_{cj} T_{ij})^{0.5} (1 - K_{ij})$$

This equation can be used with both liquid and vapor phase.

For liquid phase,

$$\frac{HL - HL^*}{RT} = ZL - 1 - \frac{AL}{BL} \left[1 - \frac{T}{a} \left(\frac{da}{dT} \right) \right] \ln \left(1 + \frac{BL}{ZL} \right) \quad 5-14)$$

$$T \left(\frac{da}{dT} \right) = \sum_i \sum_j x_i x_j m_j (a_i a_{cj} T_{ij})^{0.5} (1 - K_{ij})$$

$$HL^* = \sum_i X_i H_i^*$$

$$AL = \frac{aL^* P}{R^2 T^2}$$

$$aL = \sum_i \sum_j X_i X_j (a_i a_j)^{0.5} (1 - K_{ij})$$

$$BL = \frac{bL^* P}{RT}$$

$$bL = \sum_i X_i b_i$$

For vapor phase,

$$\frac{HV - HV^*}{RT} = ZV - 1 - \frac{AV}{BV} \left[1 - \frac{T}{a} \left(\frac{da}{dT} \right) \right] \ln \left(1 + \frac{BV}{ZV} \right) \quad 5-15)$$

$$T \left(\frac{da}{dT} \right) = \sum_i \sum_j x_i x_j m_j (a_i a_{cj} T_{ij})^{0.5} (1 - K_{ij})$$

$$HV^* = \sum_i Y_i H_i^*$$

$$AV = \frac{aV^* P}{R^2 T^2}$$

$$aV = \sum_i \sum_j Y_i Y_j (a_i a_j)^{0.5} (1 - K_{ij})$$

$$BV = \frac{bV^* P}{RT}$$

$$bV = \sum_i Y_i b_i$$

PR equation of state, from equation 4-35),

$$\frac{H - H^*}{RT} = Z - 1 - \frac{A}{2.8284B} \left[1 - \frac{T}{a} \frac{da}{dT} \right] * \ln \left[\frac{Z + 2.4142 * B}{Z - 0.4142 * B} \right]$$

$$T \left(\frac{da}{dT} \right) = \sum_i \sum_j x_i x_j m_j (a_{ci} a_{cj} T_{ij}^{0.5}) * (1 - K_{ij})$$

This equation can be used with both liquid and vapor phase.

For liquid phase,

$$\frac{HL - HL^*}{RT} = ZL - 1 - \frac{AL}{2.8284BL} \left[1 - \frac{T}{a} \frac{da}{dT} \right] * \ln \left[\frac{ZL + 2.4142 * BL}{ZL - 0.4142 * BL} \right] \quad 5-16)$$

$$T \left(\frac{da}{dT} \right) = \sum_i \sum_j x_i x_j m_j (a_{ci} a_{cj} T_{ij}^{0.5}) * (1 - K_{ij})$$

$$HL^* = \sum_i X_i H_i^*$$

$$AL = \frac{aL^* P}{R^2 T^2}$$

$$aL = \sum_i \sum_j X_i X_j (a_i a_j)^{0.5} (1 - K_{ij})$$

$$BL = \frac{bL^* P}{RT}$$

$$bL = \sum_i X_i b_i$$

For vapor phase,

$$\frac{HV - HV^*}{RT} = ZV - 1 - \frac{AV}{2.8284 BV} \left[1 - \frac{T}{a} \frac{da}{dT} \right] \ln \left[\frac{ZV + 2.4142 * BV}{ZV - 0.4142 * BV} \right]$$

5-17)

$$T \left(\frac{da}{dT} \right) = \sum_i \sum_j x_i x_j m_j (a_{ci} a_{cj} T_{rj}^{0.5})^* (1 - K_{ij})$$

$$HV^* = \sum_i Y_i H_i^*$$

$$AV = \frac{aV^* P}{R^2 T^2}$$

$$aV = \sum_i \sum_j Y_i Y_j (a_i a_j)^{0.5} (1 - K_{ij})$$

$$BV = \frac{bV^* P}{RT}$$

$$bV = \sum_i Y_i b_i$$

6. Calculate vapor flowrates on all tray, starting in the column base, using the algebraic form of the energy equation.

From equation 4-4), energy balance,

$$\frac{d(MnUn)}{dt} = L_{n+1}h_{n+1} + F_n^L h_n^F + F_{n-1}^V H_{n-1}^F + V_{n-1}H_{n-1} - V_n H_n - L_n H_n - S_n^L h_n - S_n^V H_n$$

At the column base, vapor flow rates (VB) is calculated from HL, HV and reboiler heat input, QR

$$VB = \frac{QR \times 1000000 - L(1) \times (HLB - HL(1))}{HVB - HLB}$$

At tray $N=1$ to NF , vapor flow rates (V(N)) is calculated from energy balance.

$$V(1) = \frac{HL(2) \times L(2) + HVB \times VB - HL(1) \times L(1)}{HV(1)}$$

$$V(N) = \frac{HL(N+1) \times L(N+1) + HV(N-1) \times V(N-1) - HL(N) \times L(N)}{HV(N)}$$

$$V(NF) = \frac{HL(NF+1) \times L(NF+1) + HV(NF-1) \times V(NF-1) - HL(NF) \times L(NF)}{HV(NF)}$$

At tray $N=NF+1$ to NT , vapor flow rates is calculated from the following energy balance

$$V(N) = \frac{HL(N+1) \times L(N+1) + HV(N-1) \times V(N-1) - HL(N) \times L(N)}{HV(N)}$$

$$V(NT) = \frac{HLD \times R + HV(NT-1) \times V(NT-1) - HL(NT) \times L(NT)}{HV(NT)}$$

7. Evaluate all derivatives of the component continuity equations for all NC components on all NT trays plus the reflux drum and the column base.

Total continuity equation for $N=1$ to NF tray :

$$DM(N) = L(N+1)+V(N-1)-L(N)-V(N)$$

$$DM(NF) = L(NF+1)+FL+V(NF-1)-L(NF)-V(NF)$$

Total continuity equation for $N=NF+1$ to NT tray :

$$DM(NF+1) = L(NF+2)+FV+V(NF)-L(NF+1)-V(NF+1)$$

$$DM(N) = L(N+1)+V(N-1)-L(N)-V(N)$$

$$DM(NT) = R+V(NT-1)-L(NT)-V(NT)$$

Component continuity equation for $J=1$ to NC

At column base,

$$DXB(J)/DT = [X(1,J)*L(1) - YB(J)*VB - XB(J)*B] / MB$$

At tray $N=1$ to NF ,

$$DXM(1,J)/DT = X(2,J)*L(2) + YB(J)*VB - X(1,J)*L(1) - Y(1,J)*V(1)$$

$$DXM(N,J)/DT = X(N+1,J)*L(N+1) + Y(N-1,J)*V(N-1) - X(N,J)*L(N) - V(N)*Y(N,J)$$

$$DXM(NF,J)/DT = X(NF+1,J)*L(NF+1) + Y(NF-1,J)*V(NF-1) - X(NF,J)*L(NF) - V(N)*Y(N,J) + Y(NF,J)*FL + XF(J)$$

At tray $N=NF+1$ to NT ,

$$\begin{aligned} DXM(NF+1,J)/DT &= X(NF+2,J)*L(NF+2)+Y(NF,J)* \\ &V(NF)-X(NF+1,J)*L(NF+1)-V(NF+1) \\ &*Y(NF+1,J)+FV*YF(J) \end{aligned}$$

$$\begin{aligned} DXM(N,J)/DT &= X(N+1,J)*L(N+1)+Y(N-1,J)*V(N-1)- \\ &X(N,J)*L(N)-V(N)*Y(N,J) \end{aligned}$$

$$\begin{aligned} DXM(NT,J)/DT &= XD(J)*R+Y(NT-1,J)*V(NT-1)- \\ &X(NT,J)*L(NT)-Y(NT,J)*V(NT) \end{aligned}$$

At reflux drum,

$$\begin{aligned} DXD(J)/DT &= [V(NT)*Y(NT,J)-DV*YD(J)-(R+DL)* \\ &XD(J)] / MD \end{aligned}$$

8. Integrate all ODE
9. Calculate new total liquid holdups from the sum of component holdups. Then calculate the new liquid mole fraction from the component holdups and the total holdups.
10. Calculate new liquid flow rates from the new total holdups for all trays.
11. Go back to step 4. and repeat for the next step in time.

The simplified flowchart of program is shown by Figure 5-3)

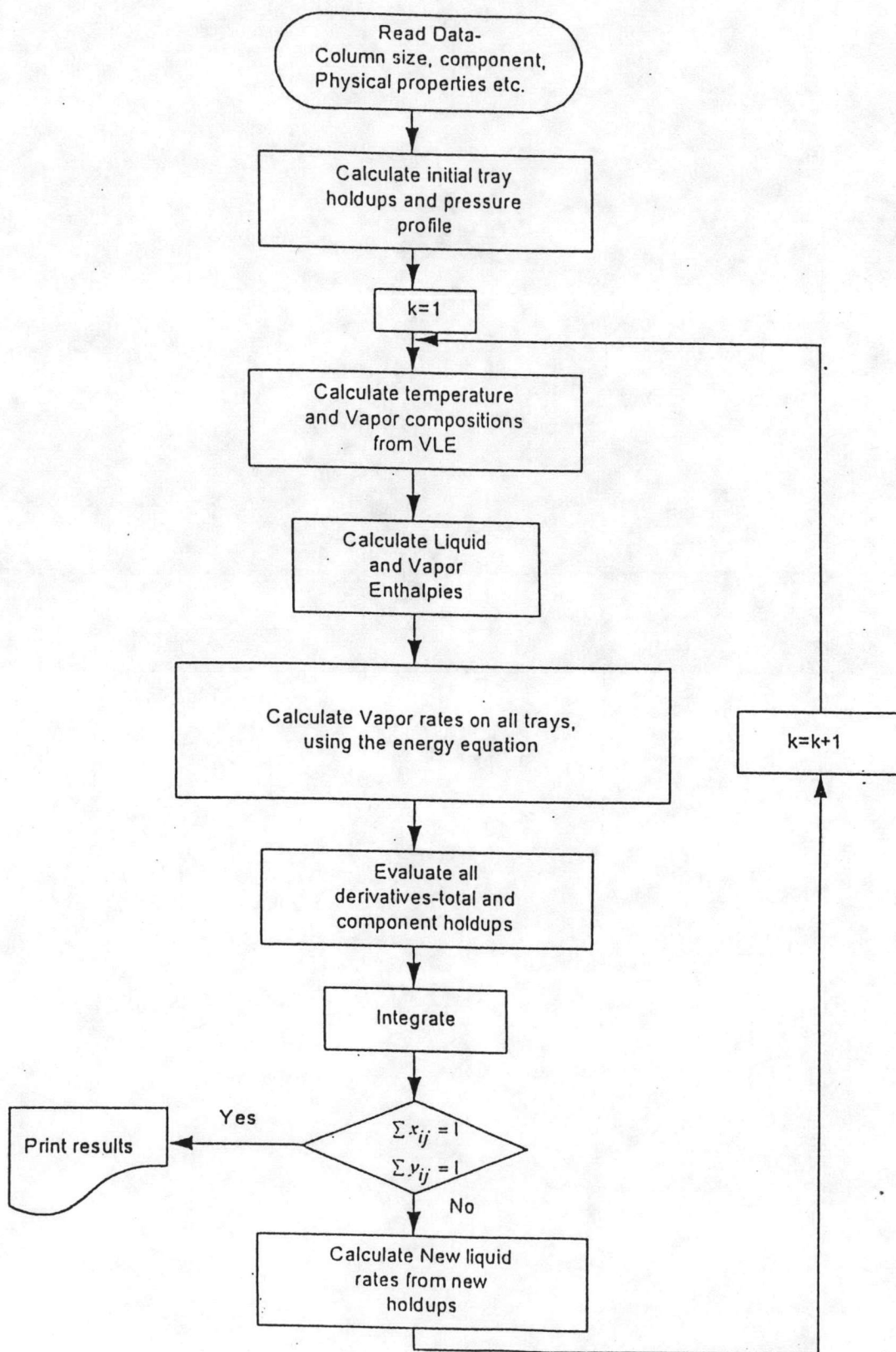


Figure 5-3 The Simplified flowchart of program

Input data required

The data required for the existing Debutanizer column design is shown in table 5-1)

Table 5-1) shows the given data which consists of :

- Characteristic of column
- Operating condition
- Feed data

Characteristic of Column			Operating Condition						
Total number of plates (NT)	=	25	Pressure in top of column, psia ,(PB)	=	126.57				
Number of trays in stripping section (NF)	=	9	Pressure in bottom of column, psia (PD)	=	133.04				
Weir height in stripping section, inch (WHS)	=	3.44	Reboiler heat-duty, Btu/hr (QR)	=	5,875,000				
Weir height in rectifying section, inch (WHR)	=	3.44	Reflux rate, lbmole/hr (R)	=	1,000.00				
Column diameter in stripping section, inch (DS)	=	72.0	Vapour product, lbmole/hr (DV)	=	0.00				
Column diameter in rectifying section, inch (DR)	=	72.0	Murphree vapor-phase efficiency	=	0.90				
Weir length in stripping section, inch (WLS)	=	51.1							
Weir length in rectifying section, inch (WLR)	=	51.1							
Volumetric holdup in column base, ft ³ (MVB)	=	130.0							
Volumetric holdup in reflux drum, ft ³ (MVD)	=	7.87							
Feed Data									
Phase	Temp. (°F)	Feed Flowrate (lbmole/hr)	Propane X ₁	Isobutane X ₂	N-Butane X ₃	Isopentane X ₄	N-Pentane X ₅	N-Hexane X ₆	
Liquid	233.62	1263.11	.3873E-1	.3772E-1	.16720	.20764	.22923	.31947	
Vapour	33.6	1.90	.1353E-1	.7596E-1	.27746	.19462	.18776	.12889	