Degrees of Freedom in Distillation

To perform a simulation of a distillation column, a set of specifications needs to be provided. To do this, one needs to understand the concept of degree of freedom. This is defined as

$$\text{Degree of Freedom} = \text{Number of unknowns} - \text{Number of equations} \quad (2\text{- }1)$$

Consider a column with N_T trays and N_C components, total condenser and total reboiler (Figure 2-1). In the case of crude, one can consider the components to be the pseudo-components that are usually generated.

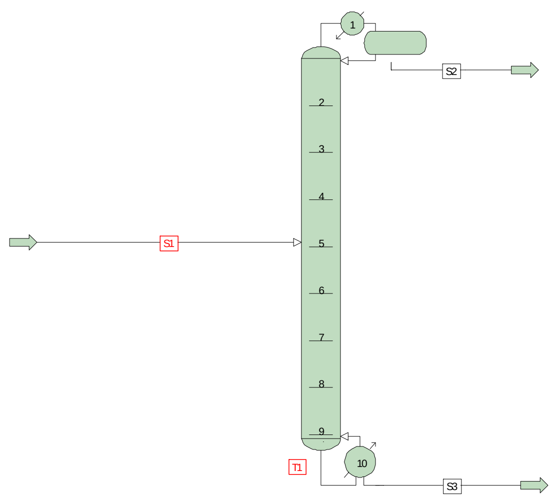

Figure 2-1: Single one-feed two product column with reboiler and condenser

VARIABLES

1) For each tray (excluding condenser and reboiler):

T_j , L_j , V_j , $x_{j,i}$, $y_{j,i}$ Variables= $3\ N_T + 2\ N_T N_C$

L= Liquid rates V= Vapor rates
x= liquid compositions y=vapor compositions
T= Tray temperatures

2) For the condenser (temperature, flows, compositions and duty)

T_C , L_0 , D , $x_{C,i}$, Q_C Variables= $N_C + 4$

D= Product Rate $\quad\quad$ Q_C = Condenser heat duty

3) For the reboiler (temperature, flows, compositions and duty)

T_R , V_{NT+1} , B , x_{Ri} , Q_R $\quad\quad$ Variables= N_C +4

B= Product Rate $\quad\quad$ Q_R = Condenser heat duty

<u>Total number of Variables</u>: **$N_T(3+2N_C)+8+2N_C$**

<u>EQUATIONS</u>:

1) Steady state mass balances for all components in all trays

$L_{j-1}\, x_{j-1,i} - [L_j\, x_{j,i} + V_j\, y_{j,i}] + V_{j+1}\, y_{j+1,i} + F_j\, z_i = 0$ $\quad\quad$ $i=1,..,N_C \quad j=1,..., N_T$

Equations: $N_C N_T$

z= feed composition $\quad\quad$ F_j= Feed rate to tray j (here we consider only one).

2) Steady state mass balances for all components the condenser

$y_{1,i} = x_{Ci}$ $\quad\quad$ $i=1,..,N_C$ $\quad\quad$ Equations: N_C

$V_1 - (L_0 + D) = 0$ $\quad\quad$ Equations: 1

3) Steady state mass balances for all components the Reboiler

$y_{NT+1,i} = x_{Ri}$ $\quad\quad$ $i=1,..,N_C$ $\quad\quad$ Equations: N_C

$L_{NT} - (V_{NT+1} + B) = 0$ $\quad\quad$ Equations: 1

4) Equilibrium Relations

$y_{j,i} = K_{j,i,}(x_j, T_j, P_j) x_{j,i}$ $\quad\quad$ $i=1,..,N_C \quad j=1,..., N_T$ $\quad\quad$ Equations: $N_T N_C$

P_j= pressures (assumed given)

5) Summation equations

$$\sum_{i=1}^{N_C} x_{j,i} = 1 \qquad j=1,\ldots, N_T$$

$$\sum_{i=1}^{N_C} x_{C,i} = 1 \qquad \text{(Condenser)}$$

$$\sum_{i=1}^{N_C} y_{j,i} = 1 \qquad j=1,\ldots, N_T$$

$$\sum_{i=1}^{N_C} y_{NT+1,i} = 1 \qquad \text{(Reboiler)}$$

6) Enthalpy balance in each tray

$$L_{j-1}\, h_{j-1} - [L_j\, h_j + V_j\, H_j] + V_{j+1} H_{j+1} + F_j\, H_{F,j} = 0 \qquad j=1,\ldots, N_T$$

h: liquid enthalpy $\quad$ H: Vapor enthalpy
H_F: Enthalpy of feed
All enthalpies are functions of composition and temperature.

7) Enthalpy balance in condenser and reboiler

$V_1\, H_1 - (L_0 + D)\, h_0 = Q_C$ $\quad$ Equations: *1*

$(L_{NT} - B)\, h_{NT} - V_{NT+1}\, H_{NT+1} = Q_R$ $\quad$ Equations: *1*

Total number of equations: $N_T(3+2N_C)+2N_C+6$

Degree of Freedom: Unknowns- Equations **= 2**

Consider now the case of a column with a total condenser and steam injection, like the one in Figure 2-2.

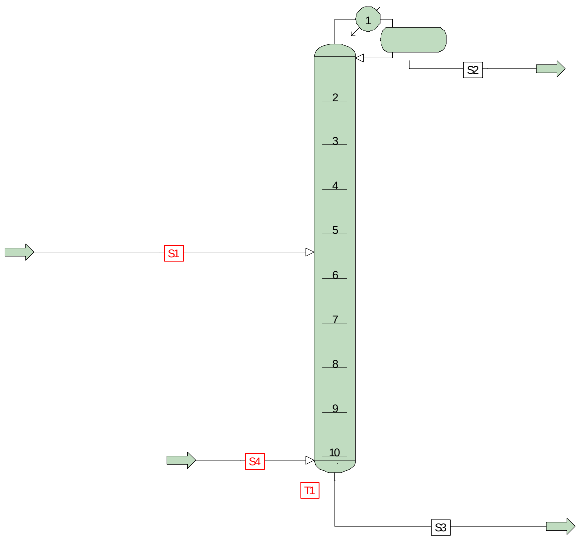

Figure 2-2: Single one-feed two product column with reboiler and condenser

Since there is no reboiler, there is N_C+4 variables less (T_R , V_{N+1}, x_{Ri} , B and Q_R). Therefore,

***<u>Total number of equations</u>*: $N_T(3+2N_C)+N_C+4$**

The number of equations is reduced by N_C+3 (N_C +1 material balances, one summation of compositions, one energy balance. Thus,

***<u>Total number of equations</u>*: $N_T(3+2N_C)+ N_C+3$**

***<u>Degree of Freedom: Unknowns- Equations</u>* = 1**