Exercise 1:

A saturated liquid mixture of components A, B, C and D is separated in a distillation column.

Data:

	z_F	x_D	x_B	Rel. vol.
A	0.3	0.95		1.25
B	0.15	0.04	0.2	1.00
C	0.3	0.01		0.6
D	0.25	0		0.4

a. Find bottom product composition and identify the key components
b. Find N_{min} from the Fenske formula
c. Find V_{min} from the Underwood formulas. The desired root is claimed by a student to be 1.0853. Is this correct?
d. How many stages and what boilup (V) would you recommend in practise?

Exercise 2:

A mixture of i-C$_4$, n-C$_4$, i-C$_5$, n-C$_5$ and n-C$_6$ is separated in a distillation column. The recovery of n-C$_4$ in the distillate is 98% and the recovery of i-C$_5$ in the bottom product is also 98%. The feed temperature is T_F=90 °C and the feed pressure P_F=6 bar.

Data:

	z_F
i-C$_4$	0.1
n-C$_4$	0.25
i-C$_5$	0.25
n-C$_5$	0.25
n-C$_6$	0.15

a. Identify the key components and find top and bottom product compositions.
b. Estimate relative volatilities based on the feed conditions.
c. What is the feed liquid fraction?
d. Find N_{min} from the Fenske formula.
e. Find R_{min} from the Underwood formula.
f. Actual reflux R=1.2 R_{min}. Use Gilliland diagram and find how many stages we need for this separation.

Exercise 1

<u>Basis 100 kmol/h</u>

a. Material balances for finding bottom compositions

$$D = 31.25 \quad , \quad B = 68.75$$

$$A : X_B^A = 0.0045$$

$$B : X_B^C = 0.432$$

$$D : X_B^D = 0.3636$$

Light key = A , Heavy key = B

b. $$S = \dfrac{\left(\dfrac{X_A}{X_B}\right)_T}{\left(\dfrac{X_A}{X_B}\right)_B} = \dfrac{\dfrac{0.95}{0.04}}{\dfrac{0.0045}{0.2}} = 1055.6$$

Fenske : $N_{min} = \dfrac{\ln S}{\ln \alpha} = \dfrac{\ln 1055.6}{\ln 1.25} \approx 31.2 = 32 \text{ stages}$

c. Underwood feed equation

$$1 - q = \sum \frac{\alpha_i z_i}{\alpha_i - \theta} \quad \overset{q=1}{=>}$$

$$0 = \frac{1.25 \cdot 0.3}{1.25 - \theta} + \frac{1 \cdot 0.15}{1 - \theta} + \frac{0.6 \cdot 0.3}{0.6 - \theta} + \frac{0.4 \cdot 0.25}{0.4 - \theta}$$

$$=> \quad \theta = 1.0853 \quad \wedge \quad \theta = 0.7610 \quad \wedge \quad \theta = 0.4512$$

but $1.25 \geqslant \theta \geqslant 1 \quad => \boxed{\theta = 1.0853}$

$$\frac{V_{T,min}}{D} = \sum_{i=A}^{C} \frac{a_i X_{i,D}}{a_i - \theta} \quad \Rightarrow \quad \underline{\text{stream}}$$

$$\frac{V_{T,min}}{D} = \frac{1.25 \cdot 0.95}{1.25 - 1.0853} + \frac{1 \cdot 0.04}{1 - 1.0853} + \frac{0.6 \cdot 0.01}{0.6 - 1.0853} + 0$$

$$\Rightarrow \boxed{V_{T,min} = 210.28 \frac{kmol}{y}}$$

b) In practise $\quad V = 1.1 \ V_{min} \ \left\{ \begin{array}{l} V = 231.3 \ kmol/y \\ N = 64 \ stages \end{array} \right.$

$\qquad\qquad\qquad\qquad N = 2 N_{min}$

Exercise 2

a. Light key : $n - C_4$

   Heavy key : $i - C_5$

   Material balances to find bottom, top compositions
   Basis 100 kmol/hr
   $$D = 35 \text{ kmol/h}$$
   $$B = 65 \text{ kmol/h}$$

b. Relative volatilities

   i) $\alpha_{ij} = \dfrac{P_i^s}{P_j^s}$: P_i^s from Antoine equation

   ii) $\alpha_{ij} = \dfrac{k_i}{k_j}$: k_i from k-value diagrams

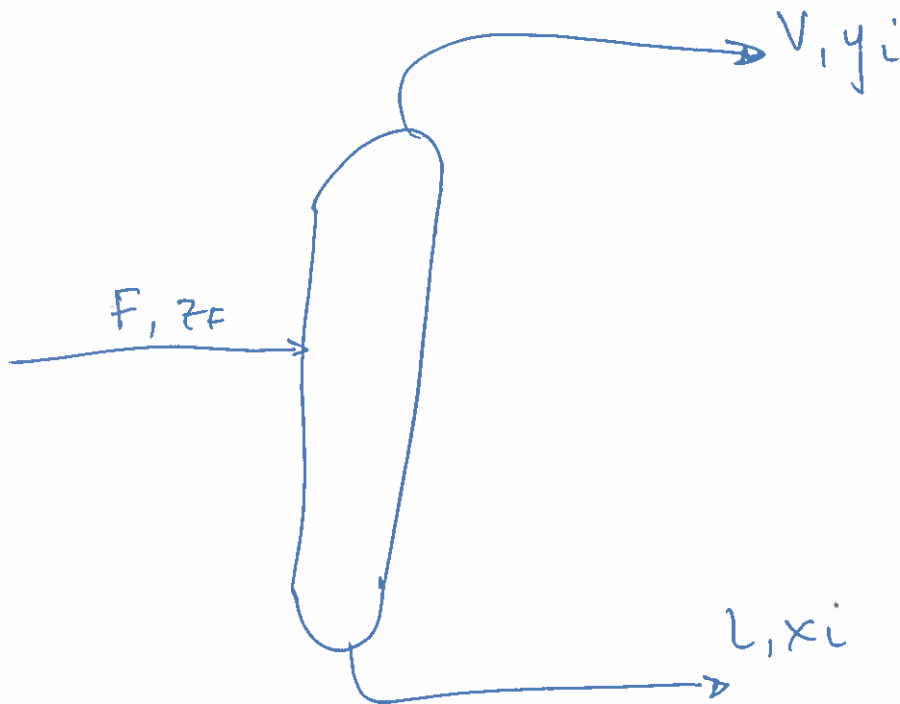 | | |
   |---|---|
   | $k_1 = 2.239$ | $\alpha_{13} = 2.359$ |
   | $k_2 = 1.809$ | $\alpha_{23} = 1.906$ |
   | $k_3 = 0.949$ | $\alpha_{33} = 1$ |
   | $k_4 = 0.791$ | $\alpha_{43} = 0.834$ |
   | $k_5 = 0.362$ | $\alpha_{53} = 0.382$ |

c. Flash calculation

$$F = V + L$$

$$Fz_i = Vy_i + Lx_i$$

$$k_i = \frac{y_i}{x_i}$$

$$Fz_i = Vy_i + L\frac{y_i}{k_i} \Rightarrow$$

$$\Rightarrow Fz_i k_i = Vy_i k_i + Ly_i \Rightarrow$$

$$\Rightarrow Fz_i k_i = Vy_i k_i + (F-V)y_i \Rightarrow$$

$$\Rightarrow y_i = \frac{Fz_i k_i}{(F-V) + Vk_i} \qquad \Rightarrow y_i = \frac{Fz_i k_i}{F + (k_i-1)V}$$

but $\sum y_i = 1 \Rightarrow$

$$\boxed{\sum \frac{Fz_i k_i}{F + (k_i-1)V} = 1}$$

$$\text{If } F=1 \Rightarrow V = 0.54 \Rightarrow \boxed{q = \frac{L}{F} = 0.46}$$

So feed is a vapor-liquid mixture.

d.

$$S = \frac{\left(\frac{x_i - c_s}{}\right)_T}{\left(\frac{x_u - c_y}{x_i - c_s}\right)_B} = \frac{\frac{0.008}{0.014}}{\frac{0.377}{}} \Rightarrow S = 2356.25$$

Fenske equation

$$N_{min} = \frac{\ln S}{\ln a_{23}} = \frac{\ln 2356.25}{\ln 1.906} \Rightarrow N_{min} = 12 \text{ stages}$$

e. Underwood formulas

$$1 - q = \sum_{u=1}^{\mu} \frac{\alpha_{uj} \, z_{u,F}}{\alpha_{uj} - \theta} \Rightarrow$$

$$\Rightarrow 1 - q = \frac{2.359 \cdot 0.1}{2.359 - \theta} + \frac{1.906 \cdot 0.25}{1.906 - \theta} + \frac{0.25}{1 - \theta} +$$

$$+ \frac{0.834 \cdot 0.25}{0.834 - \theta} + \frac{0.382 \cdot 0.15}{0.382 - \theta} \Rightarrow \boxed{\theta = 1.495}$$

$$1.906 \le \theta \le 1$$

$$R_{min} + 1 = \sum_{u=1}^{\lambda} \frac{\alpha_{uj} \, x_{u,D}}{\alpha_{uj} - \theta} \Rightarrow$$

$$\Rightarrow R_{min} + 1 = \frac{2.359 \cdot 0.286}{2.359 - 1.495} + \frac{1.906 \cdot 0.7}{1.906 - 1.495} + \frac{1 \cdot 0.014}{1 - 1.495} \Rightarrow$$

$$\Rightarrow \boxed{R_{min} = 3}$$

f. $R = 1.2 R_{min}$ => $\boxed{R = 3.6}$

$$\bar{X} = \frac{R - R_{min}}{R + 1} \quad => \bar{X} = 0.13$$

$$Y = 0.75 - 0.75 X^{0.5668} \quad => \bar{Y} = 0.514$$

$$\bar{Y} = \frac{N - N_{min}}{N + 1} \quad => \boxed{N \simeq 26 \text{ stages}}$$

Hei,

The first exercise that we would like you to start looking at is the depropanizer example described at J.C.King, Ch. 7, pg 325. We would like you to reproduce Figures 7.10, 7.11, 7.12 and 7.13.

You can use Hysys and/or Matlab. I am sending you the files in Matlab that can be used for doing this exercise along with some explanations about the files.

Try to reach me if you have any questions and problems with running the files.

Description of the case study studied in our files:

Feedrate, F=1 kmol/min
Feed liquid fraction, qF=1
Distillate flow, D=0.5 kmol/min
Bottom flow, B=0.5 kmol/min
Reflux rate, LT=2.70629 kmol/min
Boilup, VB=3.20629 kmol/min
Holdup in each stage, M=0.5 kmol
Column 'A' has:
Number of stages, NT=41
Feed stage, NF=21
Mixture to be separated
Number of components, NC= 4
Feed composition, zF=[0.25 0.25 0.25 0.25]
Relative volatilities, alpha=[3.0 2.0 1.5 1.0]

Description of the Matlab files:

multicomA: This is the main model. It can handle a column with any number of stages (NT), any number of components (NC) and assumes constant relative volatilities. In this file you have to change NT, NF, NC, alpha, Kuf, Kbf.

multicomA_LV: This is a subroutine file for simulating a column with the LV configuration. It means that we include level control of the reboiler and the condenser. In this file you have to change NT, NC, LT, VB, F, qF, zF, Ds, Bs.

running_multicomA. This is a file just for running the main model. Initial values are specified and steady state results are recorded.
In this file you have to change NT and NC.

Good luck,
Stathis

```matlab
function xprime=multicomA(t,X,U)

% **********************************************************************
% **************** Program written by Stathis Skouras at March, 2001 ****************

% **********************************************************************

% multicomA- This is a nonlinear model of a continuous distillation column with
%            NT-1 theoretical stages including a reboiler (stage 1) plus a
%            total condenser ("stage" NT. Total condenser is not an equilibrium stage).

%            Model assumptions:
%            NC components (multicomponent mixture); Component NC is the heavy
component
%            constant relative volatilities;
%            no vapor holdup;
%            one feed and two products;
%            constant molar flows ;
%            Liquid flow dynamics modelled by Franci's Weir Formula.
%            total condenser.
%
%            The model is based on column A in Skogestad and Postlethwaite
%            (1996). The model has NC*NT states.
%
% Inputs:    t    - time in [min].
%            X    - State, the first NT states are compositions of light
%                   component A, the next NT states are compositions of component B,
etc,
%                   compositions of the heavy component are not reported directly
%                   reboiler/bottom stage is stage (1) and condenser is stage (NT).
%                   The last NT states are liquid holdups in each stage.
%            U(1) - reflux L,
%            U(2) - boilup V,
%            U(3) - top or distillate product flow D,
%            U(4) - bottom product flow B,
%            U(5) - feed rate F,
%            U(6) - feed liquid fraction, qF.
%             A   - feed compositions, zF.
%          U=[U A] - Disturbances vector
% Outputs:   xprime - vector with time derivative of all the states

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%-----------------------------------------------------------------

% The following data need to be changed for a new column.
% These data are for "column A".

% Number of stages (including reboiler and total condenser:
NT=17;      % NT=18 . king uses partial reboiler (1 more stage)
% Location of feed stage (stages are counted from the bottom):
NF=10;   = 11
% End of data that have to be changed for a new column
%-----------------------------------------------------------------
% The following data need to be changed for a different mixture.
% Number of components
NC=6;
% Relative volatilities (relative to the heavy component) alpha=[alpha1
alpha2...alphaNC]
alpha=[10 2.47 1.0 0.49 0.21 0.10];    % Heavy component is n-C6 :[100 , 24.7 ,10 , 4.9 ,2.1,
% End of data that have to be changed for a different mixture
%-----------------------------------------------------------------


% Splitting the states
x=X(1:(NC-1)*NT);                      % Liquid compositions from btm to top
M=X((NC-1)*NT+1:NC*NT);                % Liquid hold up from btm to top

% Inputs and disturbances
% Inputs
LT = U(1);                             % Reflux
VB = U(2);                             % Boilup
D  = U(3);                             % Distillate
```

```
B   = U(4);                                  % Bottoms
% Disturbances
F = U(5);                                     % Feedrate
qF= U(6);                                     % Feed liquid fraction
zF= U(7:size(U,2));                           % Feed compositions

% Rearrange elements of composition vector (x) for later use
Iu=[1:NT]'*ones(1,NC-1)+NT*ones(NT,1)*[0:NC-2];
x=(x(Iu))';


% THE MODEL

% Vapour-liquid equilibria (multicomponent ideal VLE, Stichlmair-Fair, 'Distillation',
% p. 36, 1998)
y=(alpha(1:NC-1)'*ones(1,NT).*x)./(ones(1,NC-1)'*(1+(alpha(1:NC-1)-1)*x));


% Vapor Flows assuming constant molar flows
i=1:NT-1;       V(i)=VB*ones(1,NT-1);
i=NF:NT-1;      V(i)=V(i) + (1-qF)*F;


% Liquid flows are given by Franci's Weir Formula L(i)=K*Mow(i)^1.5
% Liquid flow L(i) dependent only on the holdup over the weir Mow(i)
% M(i)= Mow(i) + Muw(i) (Total holdup = holdup over weir + holdup below weir)
Muw=0.25;                                     % Liquid holdup under weir (Kmol) = half
of the nominal value
% Kuf and Kbf are based on steady state data and have to be changed for an other case
Kuf=7.2;    ⌄                                 % Constant above feed. = Ltop/(Mi-Muw)=
2.70629/(0.5-0.25)^1.5
Kbf=10.72;  ≈9.92                             % Constant below feed. = Lbottom/(Mi-Muw)=
3.70629/(0.5-0.25)^1.5
i=2:NF;        L(i)= Kbf*(M(i)-Muw).^1.5;     % Liquid flows below feed (Kmol/min)
i=NF+1:NT-1; L(i)= Kuf*(M(i)-Muw).^1.5;       % Liquid flows above feed (Kmol/min)
L(NT)=LT;                                      % Condenser's liquid flow (Kmol/min)


% Time derivatives from material balances for
% 1) total holdup and 2) component holdup

% Column
j=2:NT-1;
dMdt(j) = L(j+1)          - L(j)         + V(j-1)          - V(j);

for i=1:NC-1;
for j=2:NT-1;
dMxdt(i,j) = L(j+1)*x(i,j+1)  - L(j)*x(i,j)    + V(j-1)*y(i,j-1)       - V(j)*y(i,j);
end
end

% Correction for feed at the feed stage
% The feed is assumed to be mixed into the feed stage

dMdt(NF) = dMdt(NF)   + F;

dMxdt(:,NF)=dMxdt(:,NF)+F*zF(1:NC-1)';

% Reboiler (assumed to be an equilibrium stage)
dMdt(1) = L(2)            - V(1)        - B;

i=1:NC-1;
dMxdt(i,1)= L(2)*x(i,2) - V(1)*y(i,1) - B*x(i,1);

% Total condenser (not an equilibrium stage)
dMdt(NT) = V(NT-1)                - LT          - D;

i=1:NC-1;
dMxdt(i,NT)= V(NT-1)*y(i,NT-1) - LT*x(i,NT) - D*x(i,NT);

% Compute the derivative for the mole fractions from d(Mx) = x dM + M dx
dxdt=(dMxdt-x.*(ones(NC-1,1)*dMdt))./(ones(NC-1,1)*M');
```

```
% Rearrange elements of composition vector (dxdt) for later use
Ix=[1:(NC-1)*NT]';
W=dxdt';
dxdt=W(Ix);

% Output
xprime=[dxdt;dMdt'];
```

```
function xprime=multicomA_lv(t,X)
% multicomA_lv - Subroutine for simulation with LV-configuration.
%              It calls the model multicomA, and
%              includes control of condenser and reboiler level
%              using two P-controllers with the LV-configuration.
%
%              Inputs are reflux (LT) and boilup (VB). Disturbances
%              are feedrate and feed composition. These are set by directly
%              altering 'multicomA_lv.m'. Outputs are liquid compositions
%              for light and intermediate components and
%              liquid hold up for stages 1 through NT, given in x.

% Number of stages in the column
NT=17;    19

%Number of components
NC=6;

% Inputs and disturbances
LT=0.9;                          % Reflux
VB=0.939;  =0.839               % Boilup
F=1.0;                           % Feedrate
qF=0.34;                         % Feed liquid fraction
zF=[0.26 0.09 0.25 0.17 0.11 0.12];        % Feed compositions for component A to
component NC

% P-Controllers for control of reboiler and condenser hold up.
KcB=10;   KcD=10;               % controller gains
MDs=0.5; MBs=0.5;              % Nominal holdups - these are rather small
Ds=0.599; Bs=0.401;            % Nominal flows
MB=X((NC-1)*NT+1);   MD=X(NC*NT);   % Actual reboiler and condenser holdup
D=Ds+(MD-MDs)*KcD;             % Distillate flow
B=Bs+(MB-MBs)*KcB;             % Bottoms flow

% Store all inputs and disturbances
U(1)=LT; U(2)=VB; U(3)=D; U(4)=B; U(5)=F; U(6)=qF; A=zF; U=[U A];

xprime=multicomA(t,X,U);

t
```


$$LT=0.9=L$$

$$L' = LT + qF = 0.9 + 0.34 = 1.24$$

$$L' = B + VB \Rightarrow VB = L' - B = 1.24 - 0.401 \Rightarrow VB = 0.839$$

```
%runnning distillation model 'multicomA' for any mixture of NC components

%Number of stages
NT=17;  ≤ 15

% Number of components
NC=6;

% Initial compositions of (NC-1) components at all stages
X0=1/NC*ones(1,(NC-1)*NT);

% Initial molar holdups at all stages
M0=0.5*ones(1,NT);

% Run the model
[t,x]=ode15s('multicomA_lv',[0 20000],[X0 M0]);
lengthx=size(x);

% Vector 'Xss' returns the steady-state molar compositions of components 1 to NC-1 at
all NC stages and molar liquid hodups at all NC stages
Xss=x(lengthx(1),:)';
```
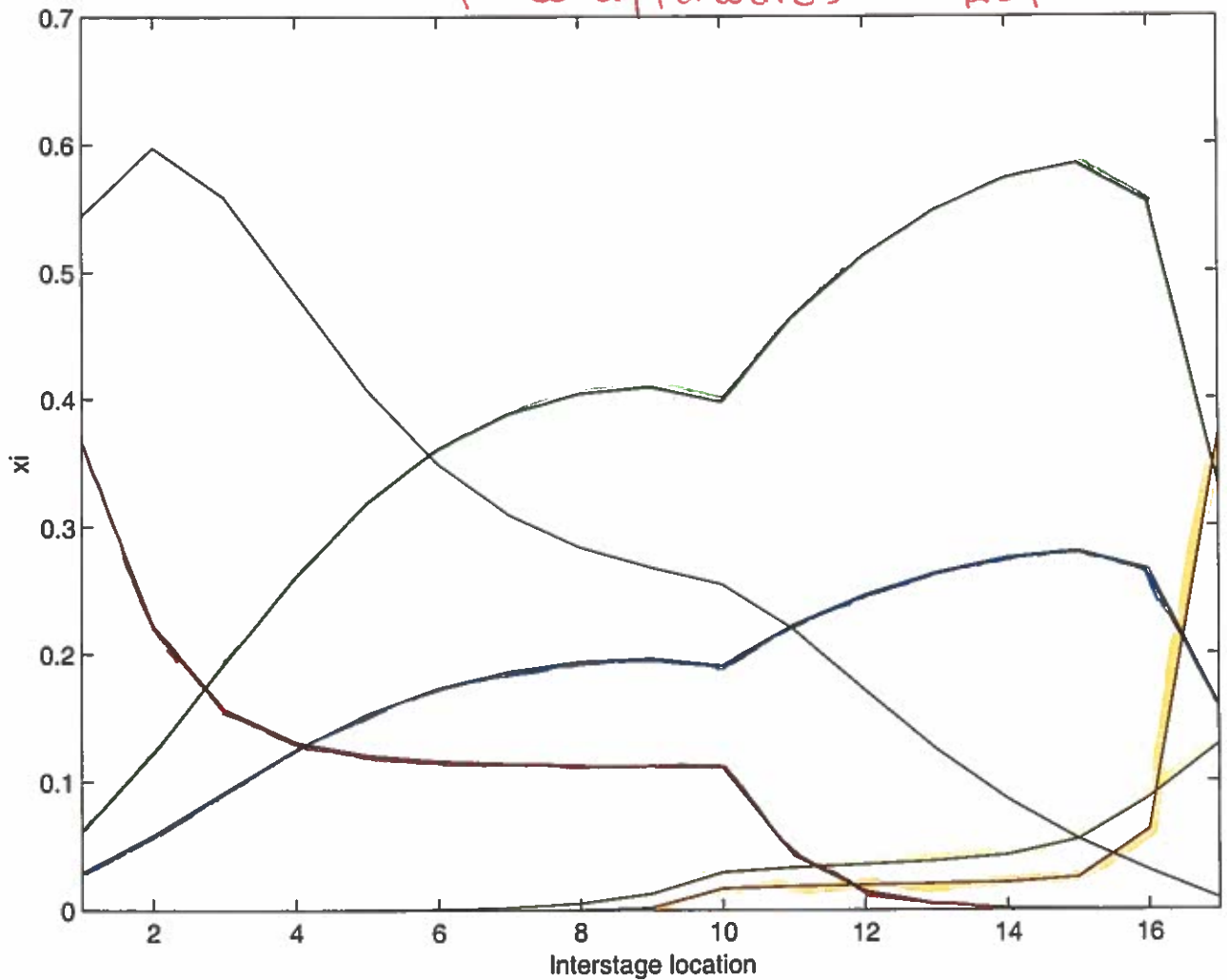
Tcbre

- The main mistake in your codes was the vector of relative volatilities, which in this files are relative to the heaviest component (n-C6)
- When you use partial condenser, like in the depropaniz we have 1 more stage in our column
- There was a small error in calculating VB and that was transferred afterwards in kbt

X₁ —
X₂ —
X₃ —
X₄ —
X₅ —
X₆ —

Bra!