CE 407 Notes // Multicomponent distillation tray-to-tray calculations

Psat_Antoine_databank.m

(See posted code.)

Psat_Antoine.m

```
function Psat = Psat_Antoine( i, T )
%saturated vapor pressures from Antoine's equation for pure substances

%components
%i =  1: methanol
%i =  2: ethanol
%i =  3: 1-propanol

if i == 1
    ii = 15;
elseif i == 2
    ii = 16;
else
    ii = 17;
end

Psat = Psat_Antoine_databank( ii , T );

end
```

f_dew.m

```
function [ T, x ] = f_dew( P, y )
%outputs: dew point temperature (degC),  liquid-phase mole fractions
%inputs:  pressure              (mm Hg),  vapor-phase mole fractions

T = fsolve(@dew,100.0);

for i = 1 : length(y)
    x(i) = y(i) * P /  Psat_Antoine(i,T);
end

    function [ lhs ] = dew( T );

    lhs = -1;
    for ii = 1 : length(y)
        lhs = lhs + y(ii) * P / Psat_Antoine(ii,T);
    end

    end

end
```

f_rop.m

```
function [ y ] = f_rop( x, xD, R )
%vapor-phase composition entering stage from liquid-phase composition
%leaving stage, distillate composition and reflux ratio by mass balances
%("R-op line equation") assuming constant molar flows

y = (R * x + xD) / (R + 1);

end
```

f_tray_to_tray_r.m

```
function [ xr, yr ] = f_tray_to_tray_r( P, xD, R, nr )
%tray-to-tray calculation for rectifying section of column
%xr(:,n) = liquid-phase composition leaving  tray n
%yr(:,n) = vapor-phase  composition entering tray n

xr = zeros(length(xD),nr);
yr = zeros(length(xD),nr);

y = xD;
for n = 1 : nr
    [ T, x ] = f_dew( P, y );
    y = f_rop( x, xD, R );
    xr(:,n) = x;
    yr(:,n) = y;
end
```

f_bubble.m

```
function [ T, y ] = f_bubble( P, x )
%outputs: bubble point temperature (degC),   vapor-phase mole fractions
%inputs:  pressure                 (mm Hg), liquid-phase mole fractions

T = fsolve(@bubble,100.0);

for i = 1 : length(x)
    y(i) = x(i) * Psat_Antoine(i,T) / P;
end

    function [ lhs ] = bubble( T );

    lhs = -1;
    for ii = 1 : length(x)
        lhs = lhs + x(ii) * Psat_Antoine(ii,T) / P;
    end

    end

end
```

f_sop.m

```
function [ x ] = f_sop( y, xB, S )
%liquid-phase composition entering stage from vapor-phase composition
%leaving stage, bottom product composition and reboil ratio by mass
%balances ("S-op line equation") assuming constant molar flows

x = (S * y + xB) / (S + 1);

end
```

f_tray_to_tray_s.m

```
function [ xs, ys ] = f_tray_to_tray_s( P, xB, S, ns )
%tray-to-tray calculation for rectifying section of column
%xs(:,n) = liquid-phase composition leaving  tray n
%ys(:,n) = vapor-phase  composition entering tray n

xs = zeros(length(xB),ns+1);
ys = zeros(length(xB),ns+1);

[ T, y ] = f_bubble( P, xB );
x = f_sop( y, xB, S );
ys(:,1) = y;
xs(:,1) = x;
for n = 1 : ns
    [ T, y ] = f_bubble( P, x );
    x = f_sop( y, xB, S );
    ys(:,n+1) = y;
    xs(:,n+1) = x;
end
```

test_Psat_Antoine.m
(Not required)

```
%boiling points
Psat_Antoine(1,64.6)
Psat_Antoine(2,78.3)
Psat_Antoine(3,97.2)

%plots of relative volatility as a function of temperature
T = linspace(60.0,100.0,9);

for i = 1 : 3
    for j = 1 : 9
        Psat(i,j) = Psat_Antoine(i,T(j));
    end
end

for i = 1 : 2
    for j = 1 : 9
        alpha(i,j) = Psat(i,j) / Psat(3,j);
    end
```

```
end

plot(T,alpha(1,:),'-r.', ...
     T,alpha(2,:),'-b.')
xlabel('{\it T} / degC')
ylabel('{\color{red} \alpha_{1,3}}, {\color{blue} \alpha_{2,3}}')
axis([60 100 1 5])
```

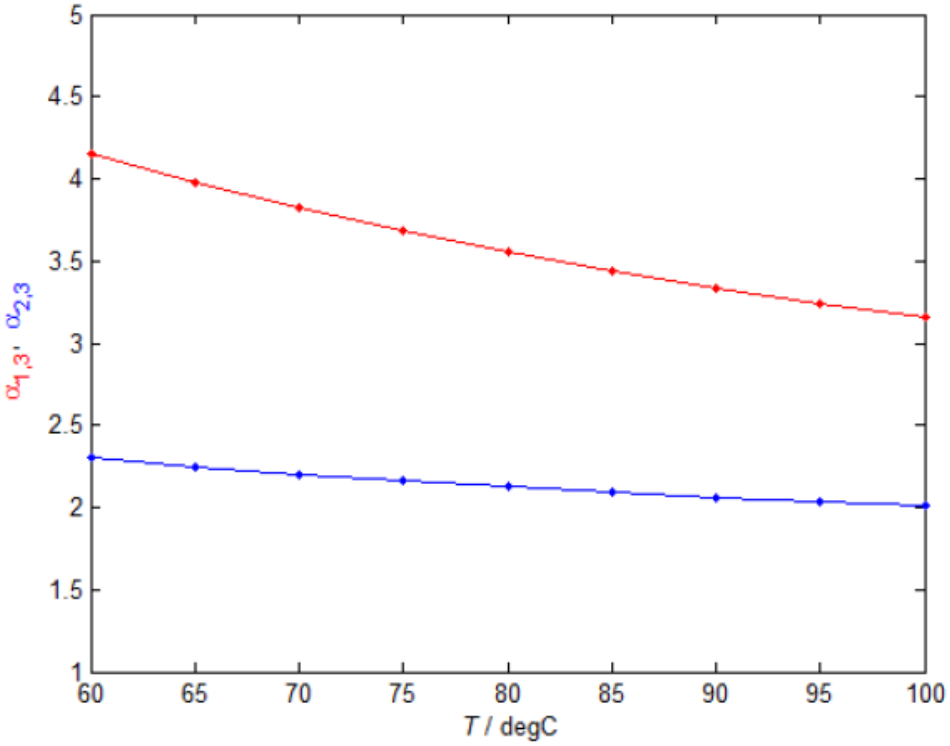
distillation_a.m

```
%%%%%%%%%%%
%%%%%%%%%%%specify distillation
%%%%%%%%%%%

%pressure
P = 760.0;

%feed
q = 1;
xF = [ 0.30, 0.25, 0.45 ];

%distillate
xD1 = 0.98;       %choice
xD3 = 5.0e-4;     %choice varies
xD = [ xD1, 1 - xD1 - xD3, xD3 ];

%bottom product
xB1 = 0.02;       %choice varies
D = (xF(1) - xB1  ) / (xD(1) - xB1);
B = (xD(1) - xF(1)) / (xD(1) - xB1);
xB3 = (xF(3) - D * xD(3)) / B;
xB = [ xB1, 1 - xB1 - xB3, xB3 ];

%reflux and reboil ratios
R = 10.0;         %choice varies
S = D / B * (R + q) + q - 1;

%%%%%%%%%%%
%%%%%%%%%%%tray-to tray-calculations
%%%%%%%%%%%

nr = 20;
[ xr, yr ] = f_tray_to_tray_r( P, xD, R, nr );
ns = 20;
[ xs, ys ] = f_tray_to_tray_s( P, xB, S, ns );

%%%%%%%%%%%
%%%%%%%%%%%display
%%%%%%%%%%%

tmp = 0:1:1;
tmp1 = 1 - tmp;

plot(tmp,tmp1,'-k', ...
     xF(1),xF(2),'rx', ...
```

```
      xD(1),xD(2),'rs', ...
      xB(1),xB(2),'r+', ...
      xr(1,:),xr(2,:),'-ks', ...
      xs(1,:),xs(2,:),'-k+')
xlabel('methanol mole fraction')
ylabel( 'ethanol mole fraction')
axis([0 1 0 1])
```

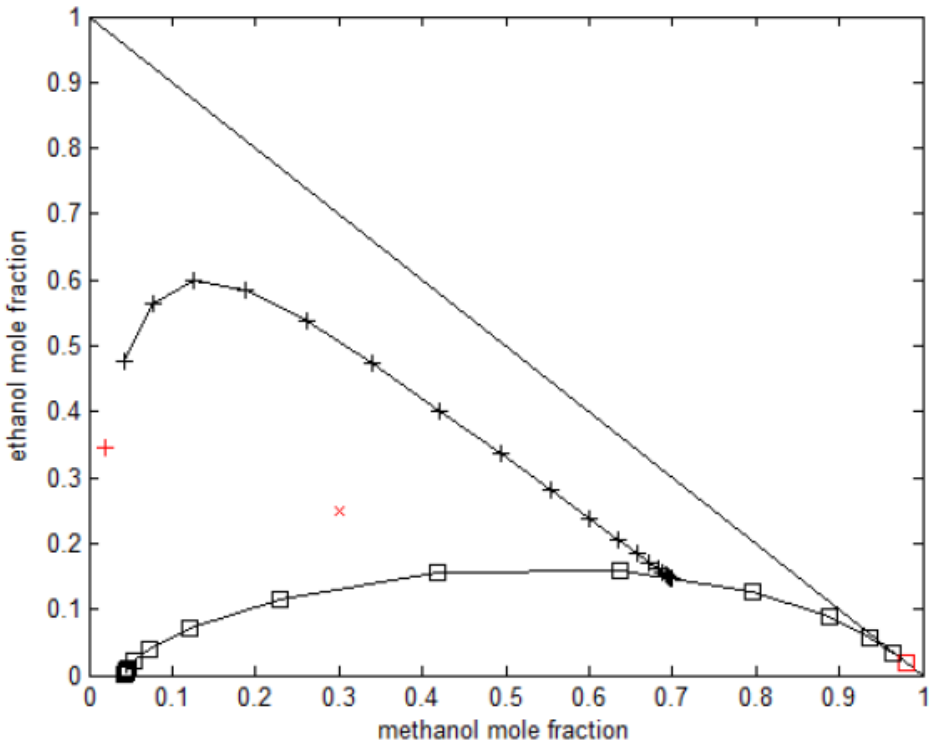
Session:

```
>> test_Psat_Antoine

ans =

  762.6743


ans =

  758.9120


ans =

  759.6616

>>
```



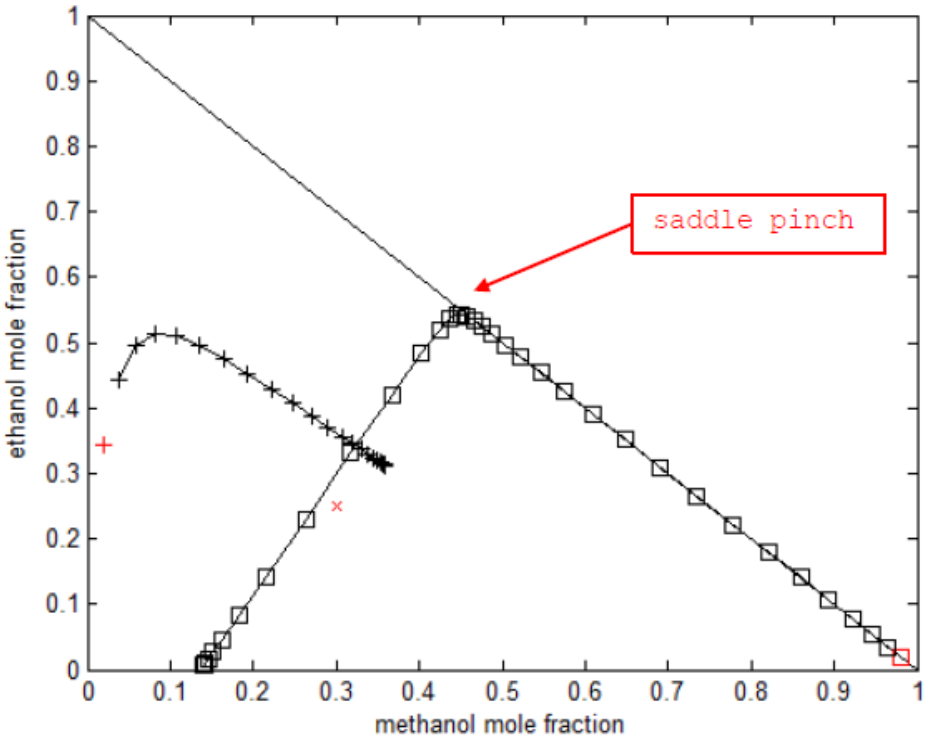
```
>> distillation_a

...

>>
```

With parameter values for Fig. 4.4(a) (not required)



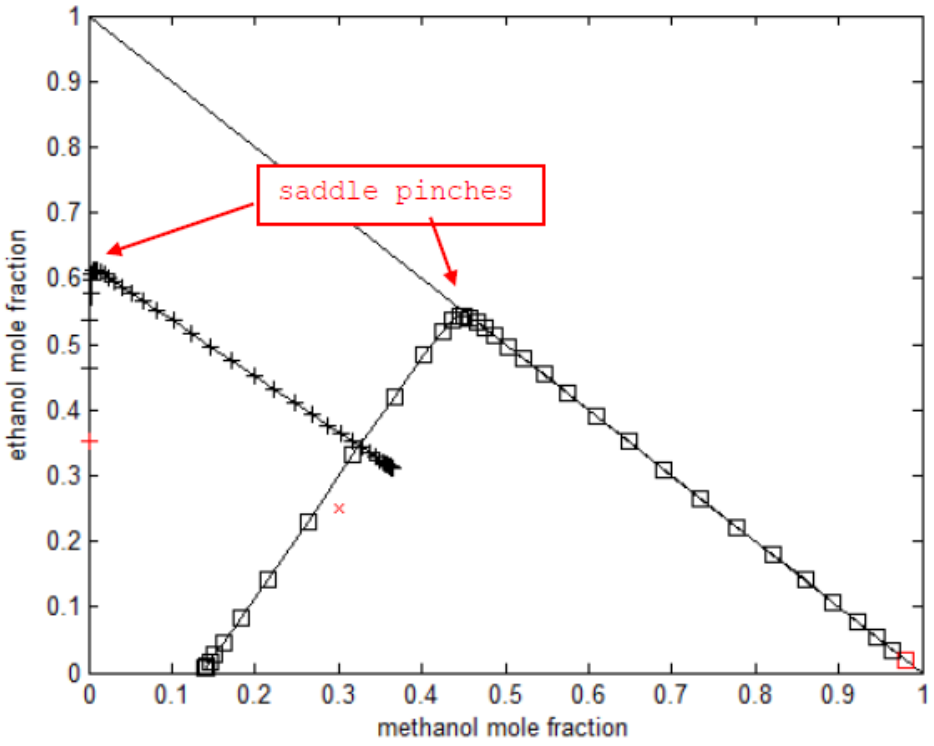
```
>> distillation_b

...

>>
```

With parameter values for Fig. 4.4(b) (required)



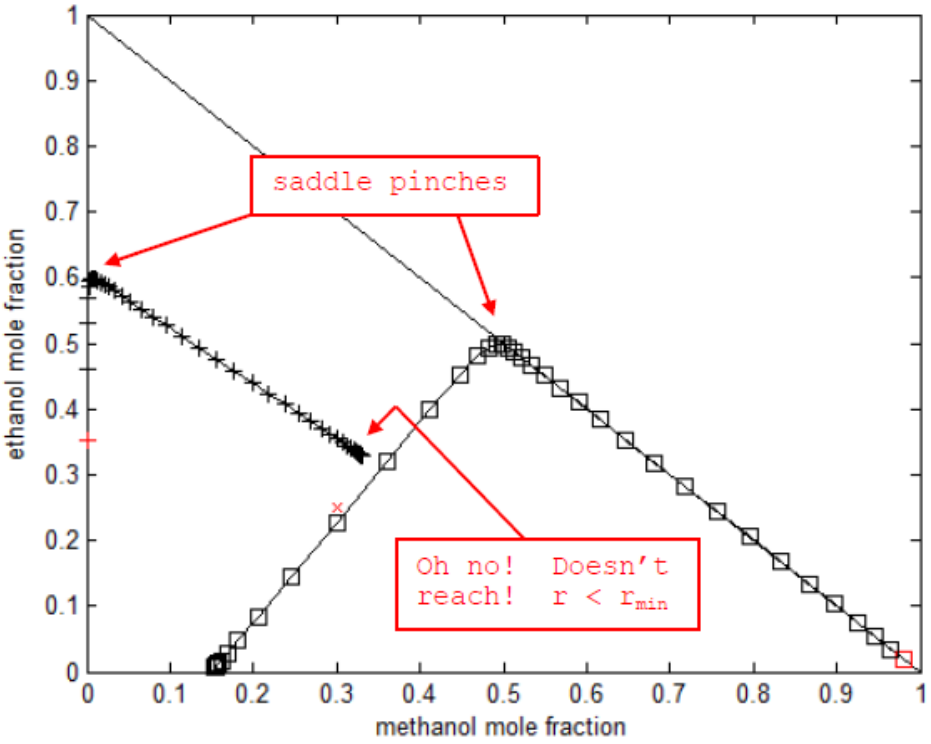
```
>> distillation_c

...

>>
```

With parameter values for Fig. 4.4(c) (not required)



```
>> distillation_d

...

>>
```

With parameter values for Fig. 4.4(d) (not required)



Comparison of cases

Figure	R	$x_{D,1}$	$x_{B,1}$	$x_{D,3}$	Comment
Figure 4.4(a)	10	0.98	0.02	5×10^{-4}	Only rectifying and stripping nodes
Figure 4.4(b)	3	0.98	0.02	5×10^{-11}	Rectifying saddle pinch
Figure 4.4(c)	3	0.98	5×10^{-4}	5×10^{-11}	Rectifying and stripping saddle pinches
Figure 4.4(d)	2.7	0.98	5×10^{-4}	5×10^{-11}	Below minimum reflux

Doherty and Malone (2001), pp. 122–123: "Figure 4.4 shows a few profiles for different values of the reflux ratio and product purities. Only nodes are evident in Fig. 4.4*a*. Figure 4.4*b* shows a rectifying sadly and Fig. 4.4*c* shows both a node and a saddle in each profile. The saddle pinches in Fig. 4.4*c* correspond to nearly infinite numbers of stages and a zone of nearly constant composition in each column section, so it may seem that this corresponds to the minimum reflux, but the reflux ration can be reduced, as shown in Fig. 4.4*d*. It is this case that corresponds to the minimum reflux (and flows). This is because the profiles do not intersect for lower values of the reflux ratio so that the product purities cannot be met even with an infinite number of stages."