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])
```

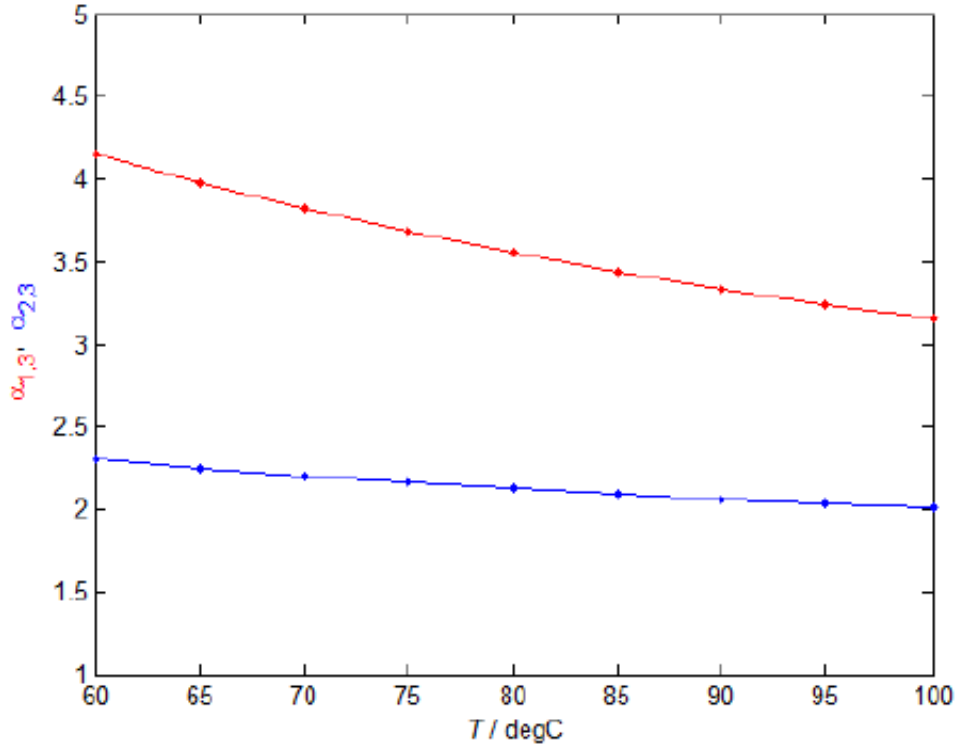
distillation.m

```
%%%%%%%%%%%
%%%%%%%%%%%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

...

>>
```