Bubble and Dew Point Calculations

These notes demonstrate bubble point and dew point calculations in Matlab.

Contents

Antoine Coefficients

The following data for methanol (MeOH) and water (H2O) are taken from Appendix B.4 of the textbook. Note that the units are assumed to be mmHg for pressure, and degrees C for temperature.

```
clear all

A.MeOH = 7.97328;
B.MeOH = 1515.14;
C.MeOH = 232.85;

A.H2O = 7.96681;
B.H2O = 1668.21;
C.H2O = 228.0;
```

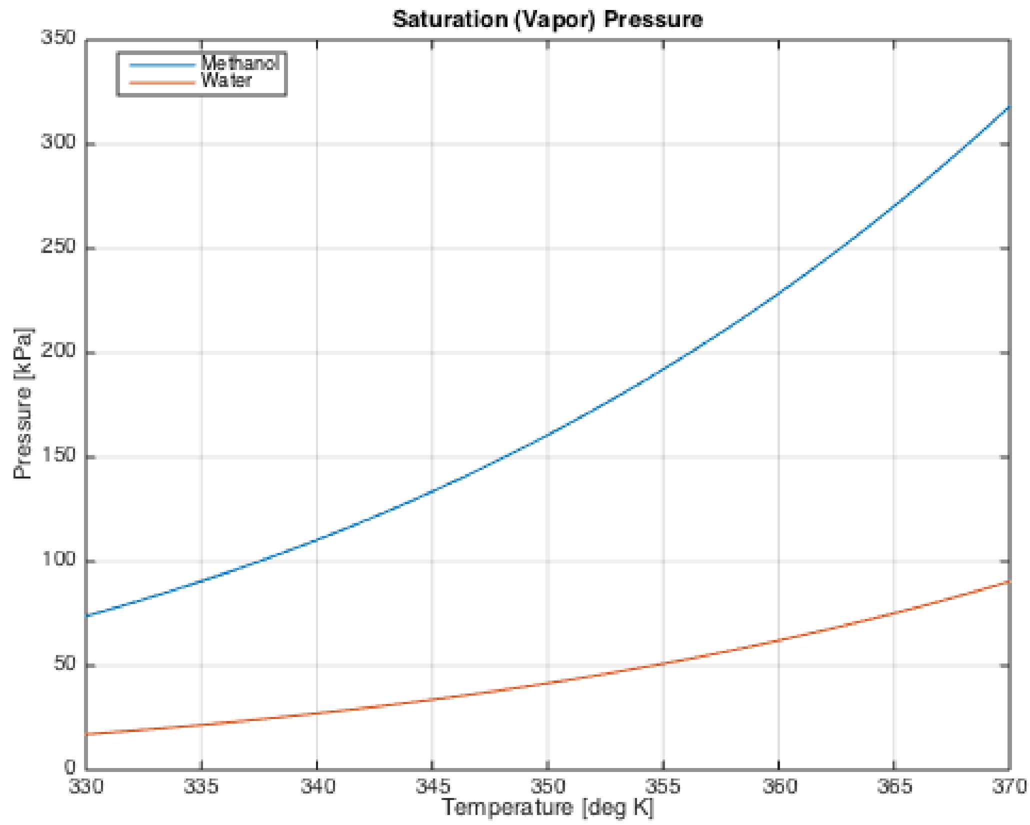
Antoine Equation

The following functions implement Antoine's equation for MeOH and H2O. The units are converted to accept temperature in degrees Kelvin and return pressure in kPa.

```
Psat.MeOH = @(T) (101.325/760)*(10.^(A.MeOH - B.MeOH/((T-273.15) + C.MeOH)));
Psat.H2O  = @(T) (101.325/760)*(10.^(A.H2O - B.H2O/((T-273.15) + C.H2O)));
```

Plot Saturate Pressure vs. Temperature

```
T = linspace(330,370,100);
plot(T,arrayfun(Psat.MeOH,T),T,arrayfun(Psat.H2O,T));
xlabel('Temperature [deg K]');
ylabel('Pressure [kPa]');
title('Saturation (Vapor) Pressure');
legend('Methanol','Water','Location','Best');
grid;
```



Boiling Points

As an initial check, we compute the boiling points of methanol and water. Here we use implement a straightforward calculation.

```
P = 101.325;

Tboil.MeOH = fzero(@(T) Psat.MeOH(T) - P, 300);
Tboil.H2O = fzero(@(T) Psat.H2O(T) - P, 300);

disp(['Boiling Points [deg K] at ',num2str(P),' kPa:']);
disp(Tboil);
```

```
Boiling Points [deg K] at 101.325 kPa:
    MeOH: 337.8258
     H2O: 373.1506
```

Bubble Point Calculations

The bubble point calculations begin by solving the equation

$$\underbrace{\sum_i x_i \frac{P_i^{sat}(T)}{P} - 1}_{f_{bub}(P,T,x)} = 0$$

```
fbub = @(P,T,x) x*Psat.MeOH(T)/P + (1-x)*Psat.H2O(T)/P - 1;
```

Given P and x, the bubble point temperature is the value of T for which

$$f_{bub}(P,T,x) = 0$$

```
P = 97.99;
x.MeOH = 0.24;

Tbub = fzero(@(T)fbub(P,T,x.MeOH),360);

disp('Bubble Point Temperature');
disp(Tbub);
```

```
Bubble Point Temperature
  358.8812
```

Once the bubble point temperature has been found, we can compute the vapor phase composition by Raoult's law

$$y_i = \frac{P_i^{sat}(T_{bub})}{P} x_i$$

```
x.H2O = 1 - x.MeOH;

y.MeOH = x.MeOH*Psat.MeOH(Tbub)/P;
y.H2O = x.H2O*Psat.H2O(Tbub)/P;
```

Display summary of results

```
disp(['Pressure: ',num2str(P),' kPa']);
disp(['Bubble Point Temperature ',num2str(Tbub),' deg K']);
disp(['Liquid Phase Composition:']);
disp(x);
disp(['Vapor Phase Composition:']);
disp(y);
```

```
Pressure: 97.99 kPa
Bubble Point Temperature 358.8812 deg K
Liquid Phase Composition:
    MeOH: 0.2400
     H2O: 0.7600

Vapor Phase Composition:
    MeOH: 0.5387
     H2O: 0.4613
```

Dew Point Calculations

The dew point calculations begin by solving the equation

$$\underbrace{\sum_i y_i \frac{P}{P_i^{sat}(T)} - 1}_{f_{dew}(P,T,y)} = 0$$

```
fdew = @(P,T,y) y*P/Psat.MeOH(T) + (1-y)*P/Psat.H2O(T) - 1;
```

Given P and y, the dew point temperature is the value of T for which

$$f_{dew}(P,T,y) = 0$$

```
P = 97.99;
y.MeOH = 0.4;

Tdew = fzero(@(T) fdew(P,T,y.MeOH),360);

disp('Dew Point Temperature');
disp(Tdew);
```

```
Dew Point Temperature
  362.9567
```

Once the dew point temperature has been determined, the liquid phase composition is found from Raoult's law

$$x_i = y_i \frac{P}{P_i^{sat}(T_{dew})}$$

```
y.H2O = 1 - y.MeOH;

x.MeOH = y.MeOH*P/Psat.MeOH(Tdew);
x.H2O = y.H2O*P/Psat.H2O(Tdew);
```

Display summary of results

```
disp(['Pressure: ',num2str(P),' kPa']);
disp(['Dew Point Temperature ',num2str(Tdew),' deg K']);
disp(['Liquid Phase Composition:']);
disp(x);
disp(['Vapor Phase Composition:']);
disp(y);
```

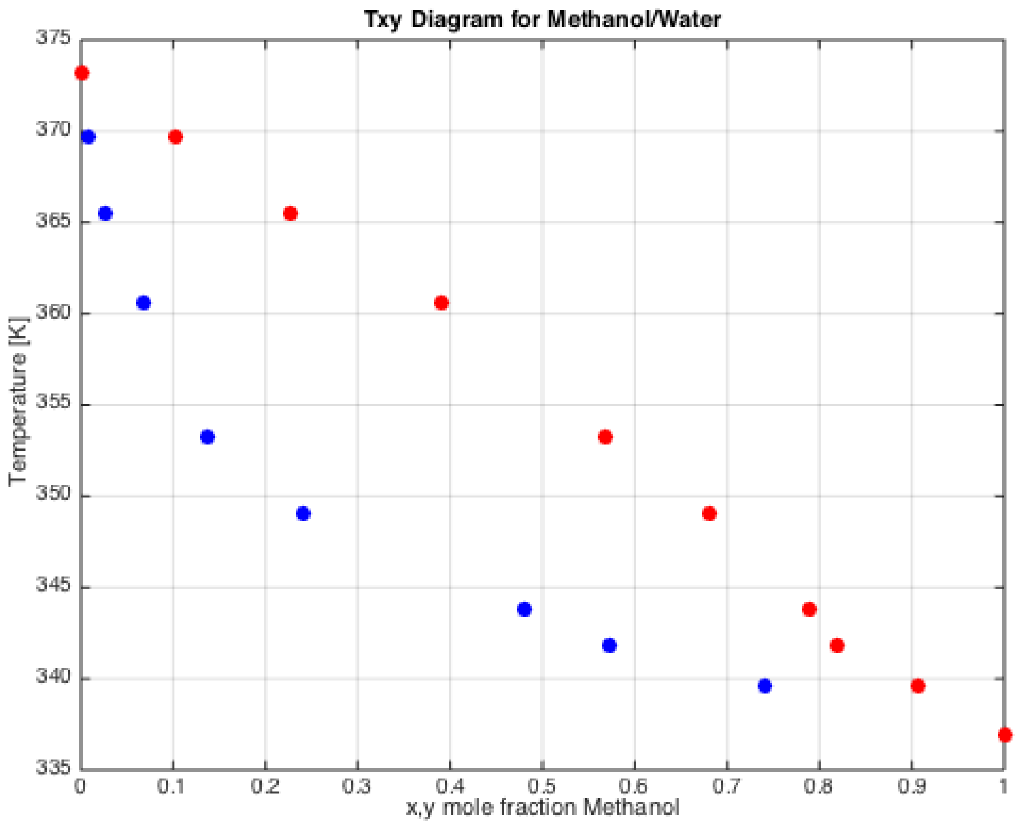
```
Pressure: 97.99 kPa
Dew Point Temperature 362.9567 deg K
Liquid Phase Composition:
```

```
    MeOH: 0.1552
     H2O: 0.8448

Vapor Phase Composition:
    MeOH: 0.4000
     H2O: 0.6000
```

Txy Diagram

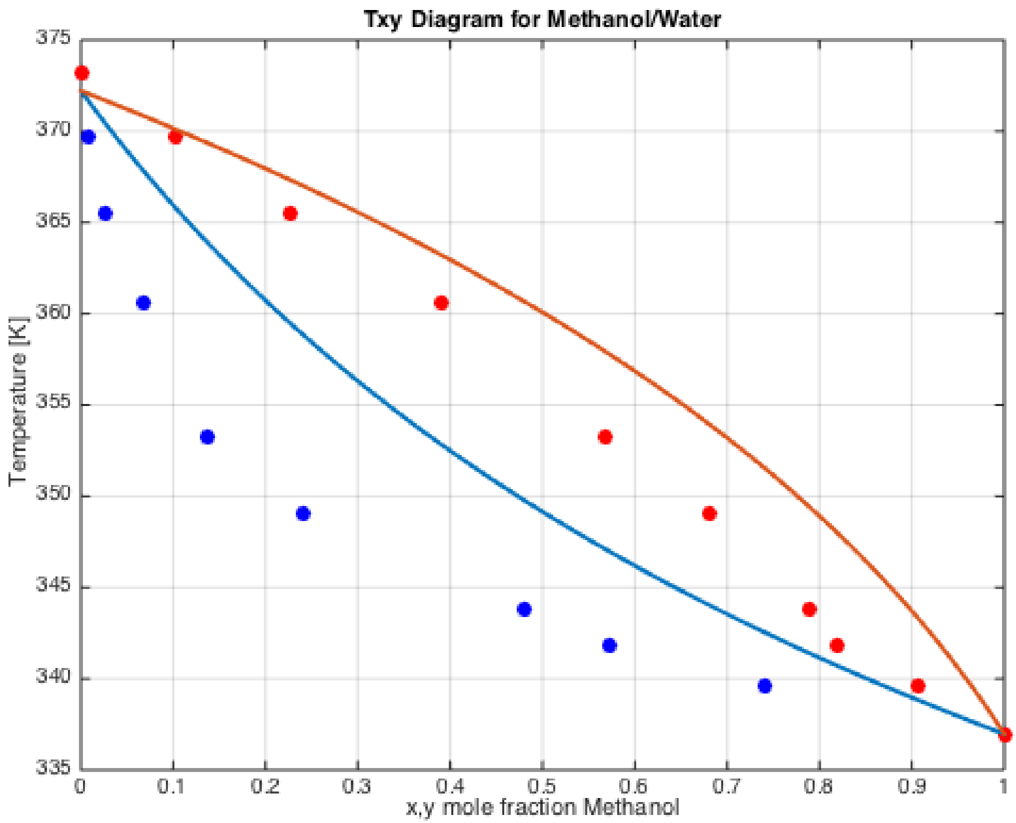
Vapor/Liquid Equilibrium data is commonly displayed in the form of a T-x-y diagram. For example, the following experimental data for a binary Methanol/Water system is available from `http://www.ddbst.com/en/EED/VLE/VLE%20Methanol%3BWater.php`

```
% Experimental Data
P = 97.99;
Texpt = [373.22 369.65 365.45 360.65 353.25 349.05 343.75 341.85 339.55 336.98];
xexpt = [0.0000 0.0084 0.0258 0.0680 0.1370 0.2400 0.4800 0.5720 0.7410 1.0000];
yexpt = [0.0000 0.1030 0.2270 0.3910 0.5680 0.6800 0.7900 0.8200 0.9060 1.0000];

plot(xexpt,Texpt,'b.','Markersize',25);
hold on;
plot(yexpt,Texpt,'r.','Markersize',25);
grid;
xlabel('x,y mole fraction Methanol');
ylabel('Temperature [K]');
title('Txy Diagram for Methanol/Water');
```



Given pressure and the liquid (or vapor) composition, we can solve for the bubble (or dew) point temperature. We

```
% Add our calculations

P = 97.99;
Tbub = @(x) fzero(@(T) fbub(P,T,x), 360);
Tdew = @(y) fzero(@(T) fdew(P,T,y), 360);

x = linspace(0,1,100);
plot(x,arrayfun(Tbub,x),'Linewidth',2)

y = linspace(0,1,100);
plot(y,arrayfun(Tdew,y),'Linewidth',2);
hold off;
```



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