Homework 6

Problem 1.1

Determine the dew point temperature and composition of the first droplet for a mixture of 70% methanol. </br></br> </br></br> Vapor-Liquid Equilibrium Data for Methanol(A) and Water(B)

Temp \degreeC	y_A	x_A
64.5	1.000	1.000
66.0	0.958	0.900
69.3	0.870	0.700
73.1	0.779	0.500
78.0	0.665	0.300
84.4	0.517	0.150
93.5	0.230	0.040
100.0	0.000	0.000

The data in the table above shows the bubble and dew lines for the methanol-water system. The temperature is the bubble or dew point temperature at a specific composition. </br></br> Using this data, the dew point temperature at 70% methanol is found by determining the temperature when $y_A = 0.70$. The composition of the first droplet is then found by determining x_A at the dew point temperature. </br></br> The code below interpolates to find T when $y_A = 0.70$ and then x_A at T scipy.interpolate.interp1d

In [ ]:

```
import matplotlib.pyplot as plt
import numpy as np
from scipy.interpolate import interp1d

molFrac = np.linspace(0,1,9999)                                     #array of

T = np.array([64.5,66,69.3,73.1,78,84.4,89.3,93.5,100])             #temp dat
yA = np.array([1,.958,.87,.779,.665,.517,.365,.23,0])               #sat vap
xA = np.array([1,.9,.7,.5,.3,.15,.08,.04,0])                        #sat liq

interpX = interp1d(xA,T,kind='cubic')
interpY = interp1d(yA,T,kind='cubic')
interpTx = interp1d(T,xA,kind='cubic')
interpTy = interp1d(T,yA,kind='cubic')
```

In [ ]:

```
mix = 0.7                                                       #mix comp
Tdew = interpY(mix)                                             #dew point te

TdewApprox = []                                                 #this loop fi
for i in interpX(molFrac):
```

```
    if i <=Tdew and i >Tdew-0.1:
        TdewApprox.append(i)

xDew = molFrac[interpX(molFrac).tolist().index(max(TdewApprox))]        #comp of firs
print('T_dew =',Tdew)
print('x_dew =',xDew)
```

```
T_dew = 76.46925604119907
x_dew = 0.35247049409881975
```

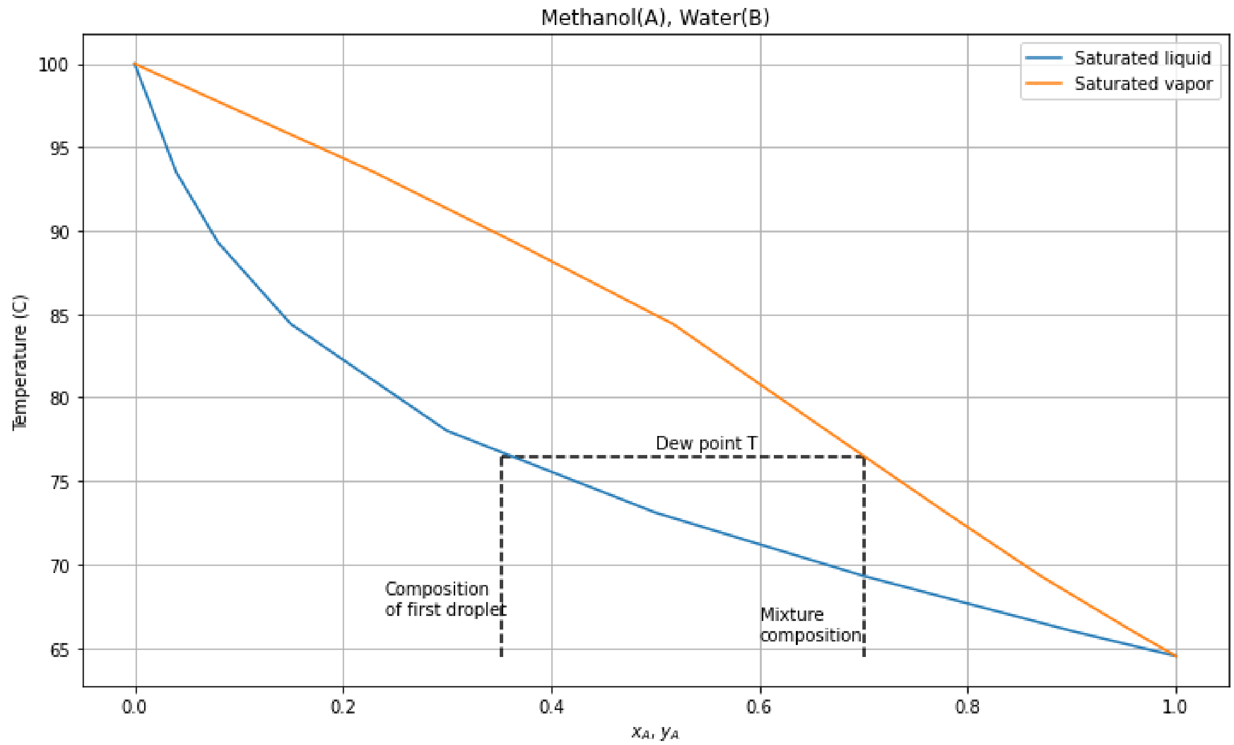
The dew point temperature is about $76.5\degree C$ and the composition of the first droplet is about 36% Methanol. </br></br> Below is the solution represented graphically

In [ ]:

```
plt.figure(figsize=(12,7))
plt.plot(xA,T,label='Saturated liquid')
plt.plot(yA,T,label='Saturated vapor')

plt.vlines(mix,min(T),Tdew,linestyles='--',color='k')
plt.vlines(xDew,min(T),Tdew,linestyles='--',color='k')
plt.hlines(Tdew,xDew,mix,linestyles='--',color='k')


plt.text(.5,77,'Dew point T')
plt.text(.24,67,'Composition\nof first droplet')
plt.text(.6,65.5,'Mixture\ncomposition')
plt.xlabel(r'$x_A$, $y_A$')
plt.ylabel('Temperature (C)')
plt.grid()
plt.title('Methanol(A), Water(B)')
plt.legend()



;
```

Out[ ]:

```
''
```



Problem 1.2

Determine the bubble point temperature when $x_A = 0.70$ and the composition of the first bubble </br></br> Following similar logic as problem 1.1, the bubble point temperature can be found by using the data provided to determine T when $x_A = 0.70$. The composition of the first bubble is y_A at the bubble point temperature. Since there is a data point for $x_A = 0.70$, no interpolation is necessary </br></br> The bubble point temperature is $69.3\degree C$ and the compostion of the first bubble is 87.0%.

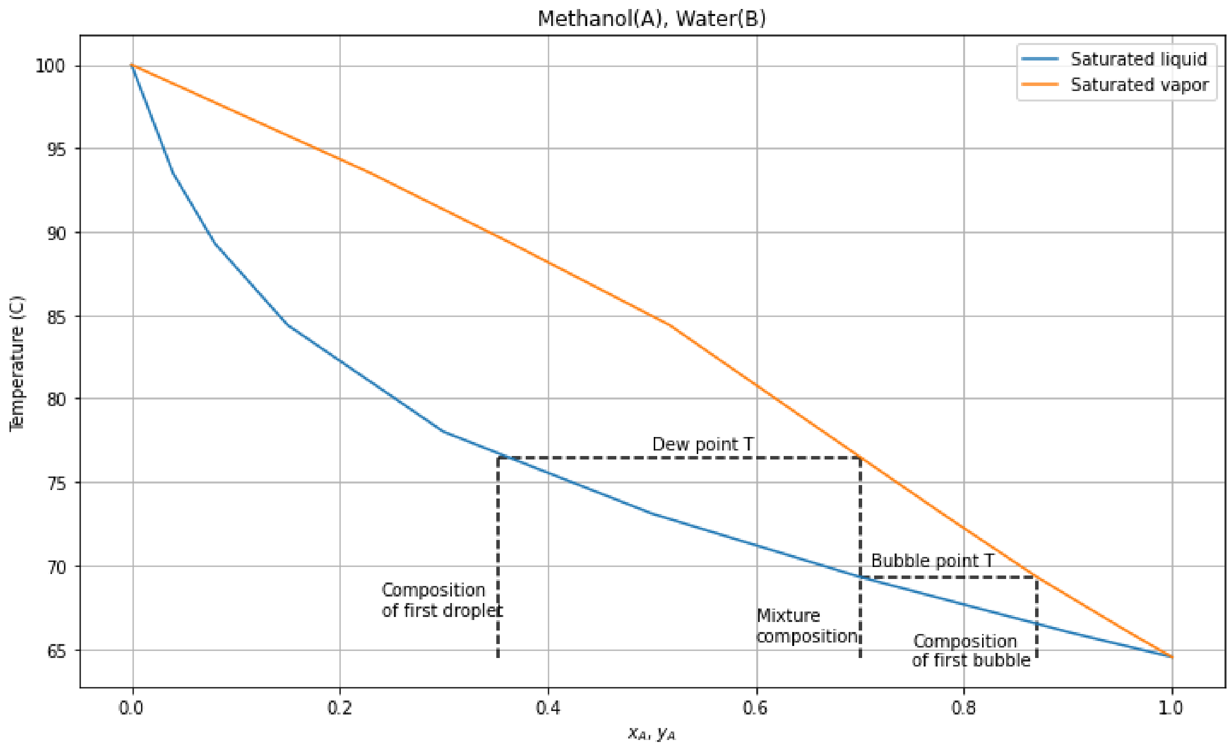
Below is the graphical representation of the solution along with the solution from problem 1.1

In [ ]:
```
Tbub = 69.3
ybub = 0.87
```

In [ ]:
```
plt.figure(figsize=(12,7))
plt.plot(xA,T,label='Saturated liquid')
plt.plot(yA,T,label='Saturated vapor')

plt.vlines(mix,min(T),Tdew,linestyles='--',color='k')
plt.vlines(xDew,min(T),Tdew,linestyles='--',color='k')
plt.hlines(Tdew,xDew,mix,linestyles='--',color='k')

plt.hlines(Tbub,mix,ybub,linestyles='--',color='k')
plt.vlines(ybub,min(T),Tbub,linestyles='--',color='k')

plt.text(.5,77,'Dew point T')
plt.text(.24,67,'Composition\nof first droplet')
plt.text(.6,65.5,'Mixture\ncomposition')
plt.text(.71,70,'Bubble point T')
plt.text(.75,64,'Composition\nof first bubble')
```

```
plt.xlabel(r'$x_A$, $y_A$')
plt.ylabel('Temperature (C)')
plt.grid()
plt.title('Methanol(A), Water(B)')
plt.legend()


;
```

Out[ ]: ''



Problem 1.3

Determine the temperature and composition of each phase when the mixture is is 70% methanol and 80% vapor </br></br> Using the inverse lever arm rule,

$$\frac{V}{V+L} = \frac{composition_{mix} - x_A}{y_A - x_A} = 0.80 = \frac{0.70 - x_A}{y_A - x_A} \tag{1}$$

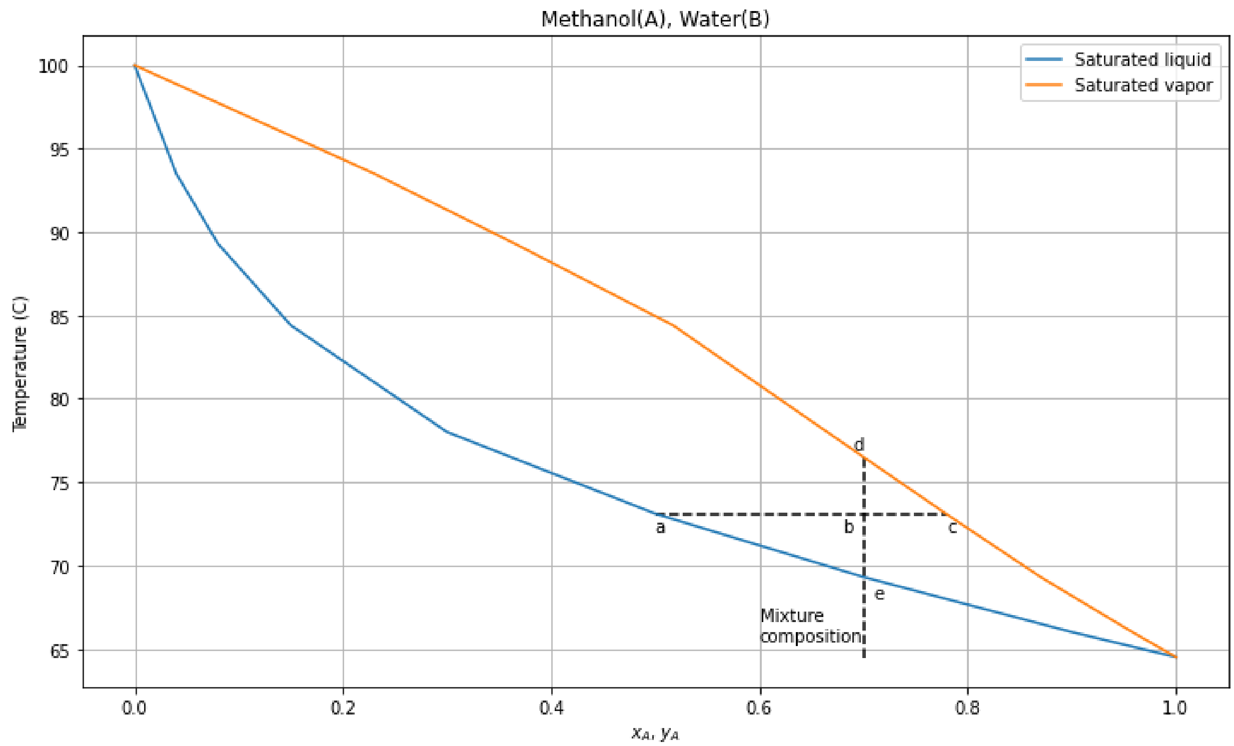
where V and L are the relative amounts of vapor and liquid respectively, x_A is the point on the saturated liquid line at a specified temperature and y_A is the point on the saturated vapor line at the same temperature. Below is a graphical representation

In [ ]:

```
plt.figure(figsize=(12,7))
plt.plot(xA,T,label='Saturated liquid')
plt.plot(yA,T,label='Saturated vapor')

plt.vlines(mix,min(T),Tdew,linestyles='--',color='k')
plt.hlines(73.1,.5,.779,linestyles='--',color='k')


plt.text(.6,65.5,'Mixture\ncomposition')
```

```
plt.text(.5,72,'a')
plt.text(.68,72,'b')
plt.text(.78,72,'c')
plt.text(.69,77,'d')
plt.text(.71,68,'e')
plt.xlabel(r'$x_A$, $y_A$')
plt.ylabel('Temperature (C)')
plt.grid()
plt.title('Methanol(A), Water(B)')
plt.legend()

;
```

Out[ ]: ''



In the diagram, $\bar{ac}$ is relative and is not necessarily the correct temperature. a represents the liquid composition and c represents the vapor composition. To find the correct temperature, (1) needs to be solved as

$$0.8 = \frac{b-a}{c-a}$$

where $b = 0.70$ </br></br> This is one equation with two unknowns but since the total composition is 0.70, it is known that y_A in (1) must correlate with a temperature in between points d and e. The following code solves (1) using the interpolated set of data.

In [ ]:

```
possibY = []                                              #loop to make array of po
for i in range(len(molFrac)):
    if molFrac[i] < ybub and molFrac[i] > mix:
        possibY.append(molFrac[i])
possibY = np.array(possibY)
possibX = interpTx(interpY(possibY))                      #possible x values
```

In [ ]:
```
sol = (mix-possibX)/(possibY-possibX)                  #solution to eq1
sol = sol.tolist()

for i in sol:                                          #loops to find x,y to ach
    if .8/i >=.9999 and .8/i <=1:
        percVap = i
        print(possibX[sol.index(i)],possibY[sol.index(i)],i)
print(interpY(possibY[sol.index(percVap)]))
```

```
0.46138061015288967 0.7596519303860773 0.8000078239522271
73.92201066046555
```

When 80% of the mixture is vapor the temperature is about $73.9\degree C$, the liquid composition is about 46.1% methanol and the vapor composition is about 76.0% methanol.

Problem 1.4

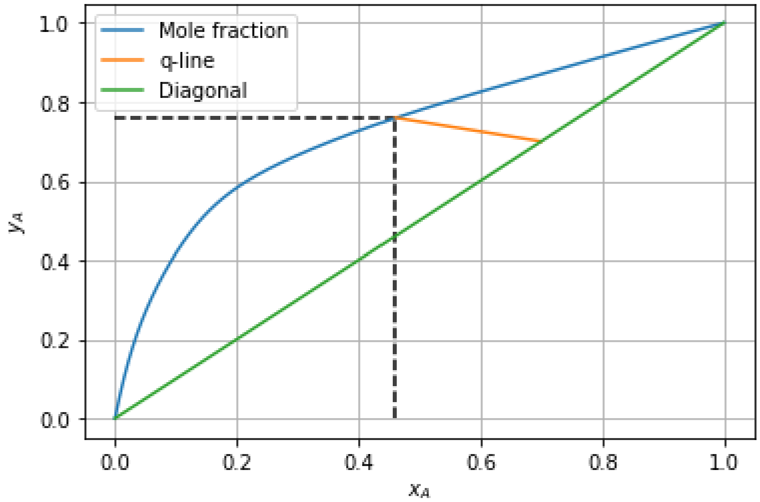
Solve problem 1.3 using the q-line </br></br> The equation for the q-line is

$$y_A = \frac{\frac{V}{F} - 1}{\frac{V}{F}} x_A + \frac{F}{V} z_A \tag{2}$$

where $\frac{V}{F} = 0.80$ and $z_A = 0.70$. The composition of each phase is found by finding where the q-line crosses the x,y curve.

In [ ]:
```
def qline(V,F,z,x):
    return (V/F-1)*F/V*x+F/V*z
plt.plot(interpTx(interpX(molFrac)),interpTy(interpX(molFrac)),label='Mole fraction')
plt.plot([.46,.7],qline(.8,1,.7,np.array([.46,.7])),label='q-line')
plt.plot([0,1],[0,1],label='Diagonal')
plt.hlines(qline(.8,1,.7,.46),0,.46,linestyles='--',color='k')
plt.vlines(.46,0,qline(.8,1,.7,.46),linestyles='--',color='k')
plt.xlabel(r'$x_A$')
plt.ylabel(r'$y_A$')
plt.grid()
plt.legend()

;
print(interpX(.46))
```

```
73.92669644249968
```



According to the q-line in the above plot, $x_A \approx 0.46$ and $y_A \approx 0.79$ which are similar to the solution found using the inverse lever-arm rule. The temperature of both phases is $73.9 \degree C$