HW 5

Problem 1.1

Plot pressure change in a system heated from 300 to 400 k that is open until all the liquid is vaporized for propane, cyclohexane, and heptane.

The change in pressure from 300 to 400 k can be found using the ideal gas law,

$$PV = nRT \tag{1}$$

This can be applied to the beginning and end of the process to give

$$P_1V_1 = n_1RT_1$$

and

$$P_2V_2 = n_2RT_2$$

Assume $V_1 = V_2$ and $n_1 = n_2$ then,

$$P_2 = \frac{P_1T_2}{T_1} \tag{1.1}$$

This relationship shows that for an ideal gas, temperature and pressure have a linear relationship.

Propane has a normal boiling point of about 231 k so it is all vapor at 300 k so the system is closed from 300 k. </br></br> cyclohexane and heptane have normal boiling points of about 354 k and 372 k respectively so the liquid for each will not completely vaporize until it reaches those temperatures so the system will be open until then and the pressure will be atmospheric pressure (1 atm).

In [ ]:

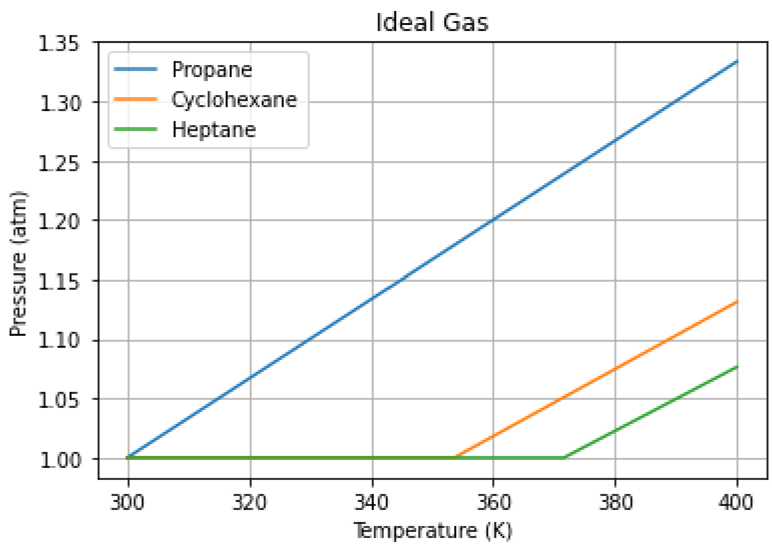
```
import numpy as np
import matplotlib.pyplot as plt
```

In [ ]:

```
bpCyc = 353.6                                                              #boil cyclohe
bpHep = 371.6                                                              #boil heptane

Tstart = 300                                                               #starting tem
Tend = 400                                                                 #end temp k
Pstart = 1                                                                 #starting pre

def gasLaw(t1,t2,p1):                                                      #calc pressur
    p2 = p1*t2/t1
    return p2


p2prop = gasLaw(Tstart,Tend,Pstart)                                     #final pressures
p2cyc = gasLaw(bpCyc,Tend,Pstart)
p2hep = gasLaw(bpHep,Tend,Pstart)
```

```
cycT = [Tstart,bpCyc,Tend]                                    #lists of tem
cycP = [Pstart,Pstart,p2cyc]

hepT = [Tstart,bpHep,Tend]
hepP = [Pstart,Pstart,p2hep]

plt.plot([Tstart,Tend],[Pstart,p2prop],label='Propane')
plt.plot(cycT,cycP,label='Cyclohexane')
plt.plot(hepT,hepP,label='Heptane')
plt.grid()
plt.legend()
plt.xlabel('Temperature (K)')
plt.ylabel('Pressure (atm)')
plt.title('Ideal Gas')



;
```

Out[ ]: ''



As illustrated by the above plot, the pressure changes linearly with temperature.

Problem 1.2

Plot pressure as a function of temperature when the species is in vapor-liquid equilibrium in a closed system.

The Antoine equation relates vapor pressure as a function of temperature,

$$P^{vap} = 10^{a-\frac{b}{T+c}} \tag{2}$$

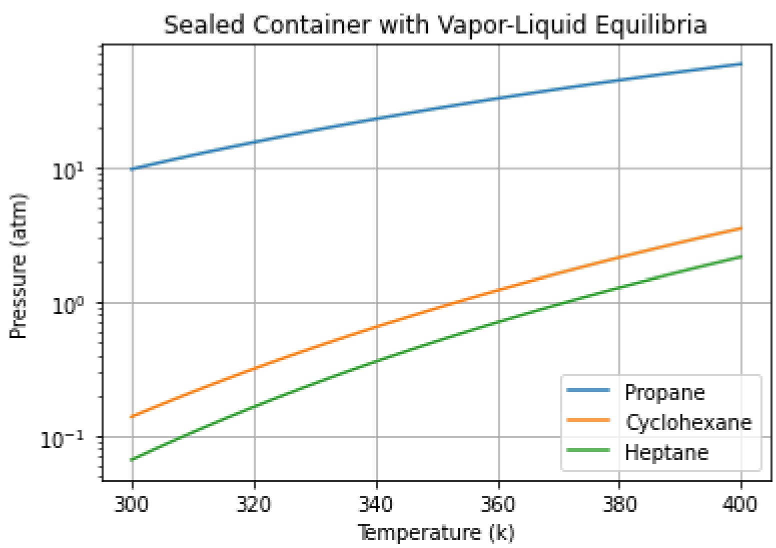
where P^{vap} is in mmHg and T is in $\degree C$ and a, b, and c are species specific constants.

In [ ]:

```
T = np.linspace(300,400)                               #temp

def antoine(a,b,c,temp):                               #temp in k
    pVap = (10**(a-b/((temp-273.15)+c)))/760           #pvap in atm
    return pVap
```

```
propA = 6.80338                                          #a,b,c for species
propB = 804
propC = 247.04

cycA = 7.264753
cycB = 1434.148
cycC = 246.7207

hepA = 6.89386
hepB = 1264.37
hepC = 216.64

plt.plot(T,antoine(propA,propB,propC,T),label='Propane')
plt.plot(T,antoine(cycA,cycB,cycC,T),label='Cyclohexane')
plt.plot(T,antoine(hepA,hepB,hepC,T),label='Heptane')
plt.yscale('log')
plt.grid()
plt.legend()
plt.xlabel('Temperature (k)')
plt.ylabel('Pressure (atm)')
plt.title('Sealed Container with Vapor-Liquid Equilibria')

;
```

Out[ ]: ''



The above plot shows a somewhat linear relationship between temperature and $\log(P)$ and the pressure increases much more dramatically than with the system with only ideal gas.