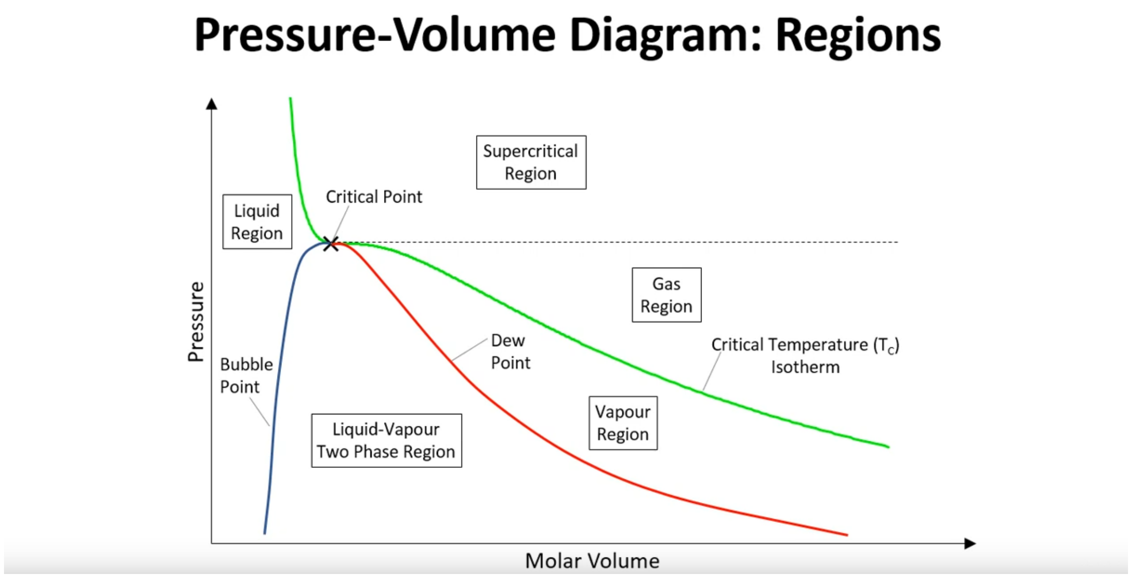
Equations_Of_State_pt1

March 19, 2023



Liquid-Vapour Two Phase Region: Coexistence of liquid and vapour, encapsulated between dew-point and bubble point line.

Vapour Region: Between Dew Point and Critical Temperature (Tc) Isotherm, where our substamce is in the gas phase but below the critical temperature

Dashed line represents the critical pressure

1 Ideal Gas Law

1.1 Assumptions:

- Volume occupied by gas molecules is negligible
- There is no intermolecular attraction or repulsion between the gas molecules

1.2 Limitations:

- Unreliable at low temperatures and/or high pressures
- Cannot predict vapour-liquid coexistence

[4]:
```
import pandas as pd
import matplotlib.pyplot as plt
```

[5]:
```
# Constant Values
R = 8.314 # cm^3 MPa / K mol
list_of_volumes = [i for i in range(30, 601, 1)]
list_of_temperatures = [255.2, 265.1, 274.4, 284.0, 294.4, 304.1, 334.1,354.1]
```

[6]:
```
critical_pressure = 7.377 # MPa
critical_volume = 94.120 # cm^3 / mol
critical_temperature = 304.128 # K
```

[7]:
```
def ideal_gas_law(gas_constant, list_of_volumes, list_of_temperatures):
    df = pd.DataFrame(columns = [str(i) for i in list_of_temperatures], index =␣
 ↪list_of_volumes)

    for index, rows in df.iterrows():
        for column in df:
            df[column][index] = (float(column) * gas_constant) / index

    return df
```

[8]:
```
ideal_gas_df = ideal_gas_law(R, list_of_volumes, list_of_temperatures)
```

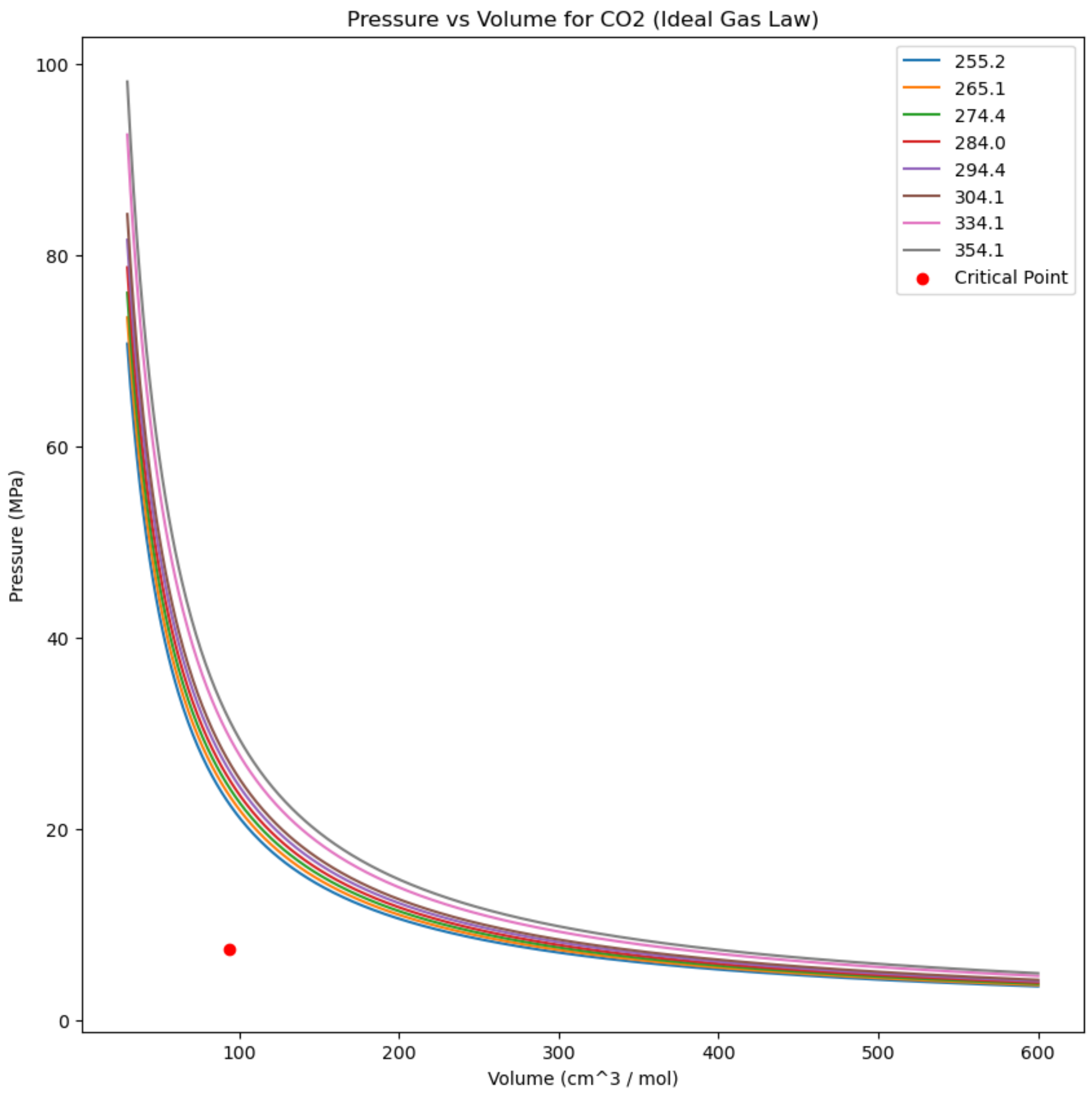
[9]:
```
ideal_gas_df
```

[9]:
```
         255.2      265.1      274.4      284.0      294.4      304.1  \
30   70.724427  73.468047  76.045387  78.705867  81.588053  84.276247
31   68.442994   71.09811   73.59231  76.166968  78.956181  81.557658
32    66.30415  68.876294   71.29255   73.78675    76.4888  79.008981
33   64.294933  66.789133   69.13217  71.550788  74.170958   76.61477
34   62.403906  64.824747  67.098871  69.446353  71.989459  74.361394
..         …          …          …          …          …          …
596   3.559954   3.698056   3.827788   3.961705   4.106781   4.242093
597   3.553991   3.691862   3.821376   3.955069   4.099902   4.234987
598   3.548048   3.685688   3.814986   3.948455   4.093046   4.227905
599   3.542125   3.679535   3.808617   3.941863   4.086213   4.220847
600   3.536221   3.673402   3.802269   3.935293   4.079403   4.213812

         334.1      354.1
30   92.590247  98.132913
31   89.603465  94.967335
32   86.803356  91.999606
33   84.172952  89.211739
34   81.697276  86.587865
..         …          …
596   4.660583   4.939576
597   4.652776   4.931302
598   4.644996   4.923056
599   4.637241   4.914837
```

```
600    4.629512    4.906646

[571 rows x 8 columns]
```

[10]:

```
# Plot each column of the dataframe as a line on the same plot with index as␣
↪x-axis and pressure as y-axis
plt.figure(figsize = (10, 10))
for column in ideal_gas_df:
    plt.plot(ideal_gas_df.index, ideal_gas_df[column], label = column)
plt.xlabel('Volume (cm^3 / mol)')
plt.ylabel('Pressure (MPa)')


#Plot the critical point as a red dot
plt.scatter(critical_volume, critical_pressure, color = 'red', label =␣
↪'Critical Point')


plt.title('Pressure vs Volume for CO2 (Ideal Gas Law)')
plt.legend()
plt.show()
```



Critical Point is for Co2 - Isotherm goes nowhere near it

2 Peng-Robinson Equation of State

Peng-Robinson equation of state

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)} \qquad a = 0.45724\frac{\alpha R^2 T_c^2}{P_c} \quad b = 0.07780\frac{RT_c}{P_c}$$

$$\alpha = \left(1+\kappa(1-\sqrt{T/T_c}\right)^2 \qquad \kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

where P is the pressure (Pa);
V is the molar volume ($\text{m}^3\ \text{mol}^{-1}$);
R is the gas constant (8.314 $\text{J mol}^{-1}\ \text{K}^{-1}$);
T is the absolute temperature (K);
P_c is the critical pressure for the component of interest (Pa);
T_c is the critical temperature for the component of interest (K);
and ω is the acentric factor for the component of interest.

Omega {w} = accentric factor, shape of the molecule. Completely spherical is 0, most noble gases

```
[11]: # Accentric factor is usually from literature
w = 0.224
kappa = 0.37464 + 1.54226 * w - 0.26992 * w**2
alpha = lambda T: (1 + kappa * (1 - (T / critical_temperature)**0.5))**2
```

```
[12]: bc = 0.07780 * R * critical_temperature / critical_pressure
print(bc)
```

```
26.666513614965435
```

```
[13]: ac = 0.45724 * R**2 * critical_temperature**2 / critical_pressure
print(ac)
```

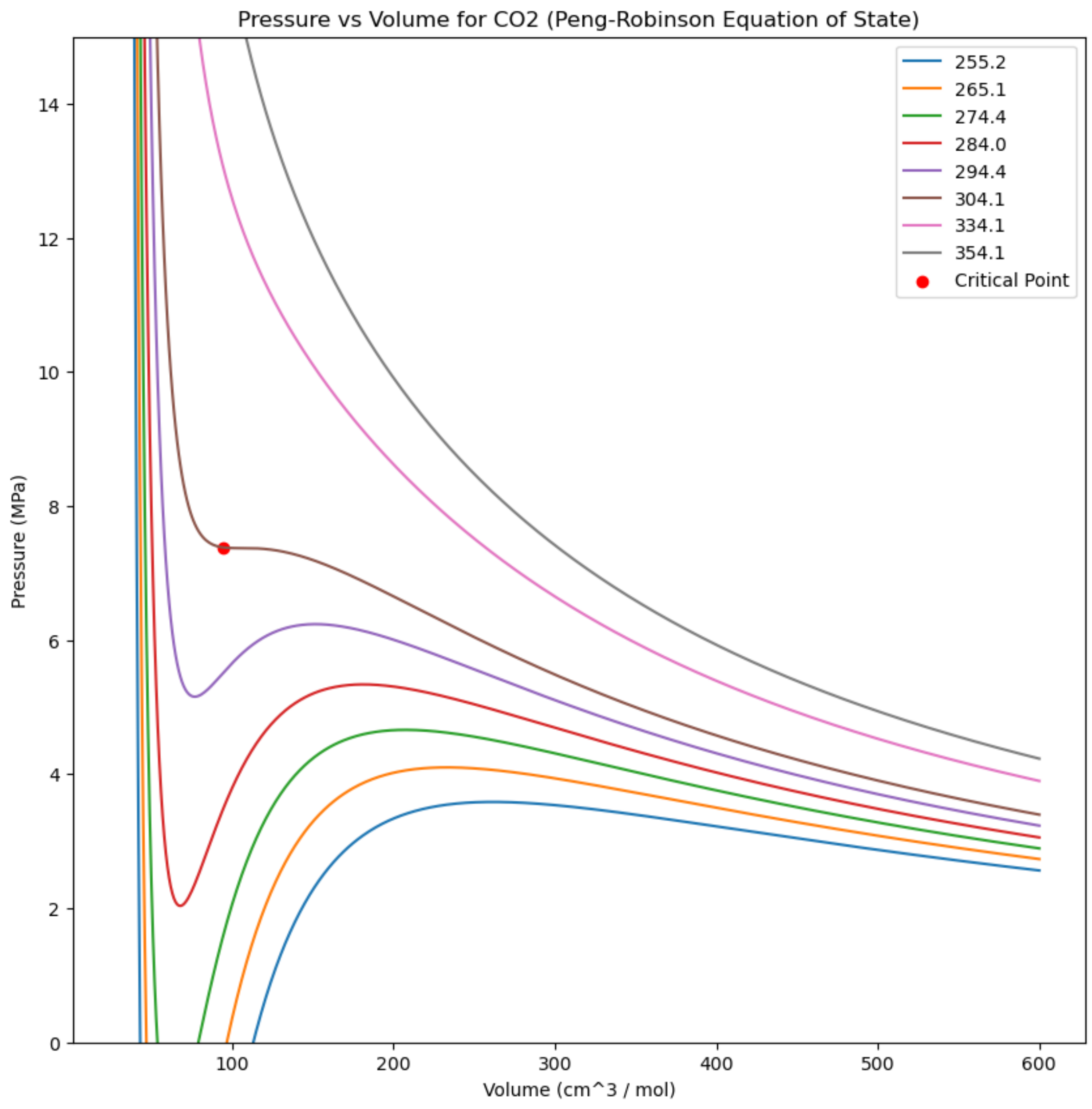
```
396275.55680960533
```

```
[14]: def peng_rob(gas_constant, list_of_volumes, list_of_temperatures,w, kappa, bc,␣
↪ac):
    df = pd.DataFrame(columns = [str(i) for i in list_of_temperatures], index =␣
↪list_of_volumes)
    temperature_aT = { T : (ac * (alpha(T))) for T in list_of_temperatures}
    for index, rows in df.iterrows():
        for column in df:
            df[column][index] = ((gas_constant * float(column)) / (index - bc))␣
↪- (temperature_aT[float(column)]/((index*(index+bc) + bc*(index-bc))))
```

```
    return df
```

[15]:
```
preos_df = peng_rob(gas_constant=R, list_of_volumes=list_of_volumes,␣
 ↪list_of_temperatures=list_of_temperatures, w=w, kappa=kappa, bc=bc, ac=ac)
```

[16]:
```
# Plot preos_df, each column of the dataframe as a line on the same plot with␣
 ↪index as x-axis and pressure as y-axis, reduce y axis from 0 to 15
# Plot the critical point as a red dot
plt.figure(figsize = (10, 10))
for column in preos_df:
    plt.plot(preos_df.index, preos_df[column], label = column)
plt.xlabel('Volume (cm^3 / mol)')
plt.ylabel('Pressure (MPa)')
plt.ylim(0, 15)
plt.title('Pressure vs Volume for CO2 (Peng-Robinson Equation of State)')
plt.scatter(critical_volume, critical_pressure, color = 'red', label =␣
 ↪'Critical Point')

plt.legend()
plt.show()
```



[17]:
```
# Find critical point for Peng-Robinson Equation of State using fsplve
from scipy.optimize import fsolve

Tc = 304.128
Pc = 7.377
R = 8.314
w = 0.224
kappa = 0.37464 + 1.54226 * w - 0.26992 * w**2
alpha = lambda T: (1 + kappa * (1 - (T / Tc)**0.5))**2

bc = 0.07780 * R * Tc / Pc
print(bc)
```

```
ac = 0.45724 * R**2 * Tc**2 / Pc
print(ac)
```

```
26.666513614965435
396275.55680960533
```

[18]:

```
from scipy.optimize import fsolve

def f(Vc):
    Pc = 7.377 # example value
    R = 8.314 # J/(mol*K)
    Tc = 304.128 # K


    A = ac * Pc / (R * Tc)**2 # calculate A using ac, Pc, R, and Tc
    #print(A)
    B = bc * Pc / (R * Tc) # calculate B using bc, Pc, R, and Tc
    #print(B)

    Z = Pc*Vc/(R*Tc)
    print(Z)
    return 1*Z**3 + (-(1-B))*(Z**2) + (A-3*B**2-2*B) * Z - (A*B-B**2-B**3)

# initial guess for Vc
Vc_guess = 0.1

# solve for Vc when f(Vc) equals 0
Vc_solution = fsolve(f, Vc_guess)

print("Vc =", Vc_solution)
```

```
[0.00029175]
[0.00029175]
[0.00029175]
[0.00029175]
[0.02946692]
[0.08781725]
[0.14460107]
[0.18368107]
[0.21428775]
[0.2371007]
[0.25446203]
[0.26762591]
[0.27772322]
[0.28561995]
[0.29210604]
[0.29810179]
```

```
[0.30564994]
[0.33179765]
[0.31052141]
[0.31052142]
[0.33969658]
[0.31284225]
[0.32013604]
[0.32269987]
[0.32126178]
[0.32139022]
[0.32137893]
[0.32137903]
[0.32137903]
Vc = [110.15498908]
```

[19]:
```
f(110.16)
```

```
0.32139364461915276
```

[19]:
```
8.53852726023785e-09
```

[23]:
```
A = ac * Pc / (R * Tc)**2
```

[25]:
```
B = bc * Pc / (R * Tc)
```

[21]:
```
import CubicEquationSolver as ces
#1*Z**3 + (-(1-B))*(Z**2) + (A-3*B**2-2*B) * Z - (A*B-B**2-B**3)
```

[38]:
```
Z_roots = ces.solve(1, -0.94805090, 0.23069070, -0.01496327)
```

[34]:
```
T = 284.00 # K
P = 4.6 # MPa
```

[39]:
```
Z_roots
```

[39]:
```
array([0.61016106, 0.10555004, 0.2323398 ])
```

[50]:
```
Vc_root1 = Z_roots[1]* R * T / P
print(f' At Z = {Z_roots[1]}, the Volume is {Vc} cm^3/mol. This is the liquid␣
 ↪phase (Plot on graph)')
```

```
 At Z = 0.10555004295080034, the Volume is 119.25981783492531 cm^3/mol. This is
the liquid phase (Plot on graph)
```

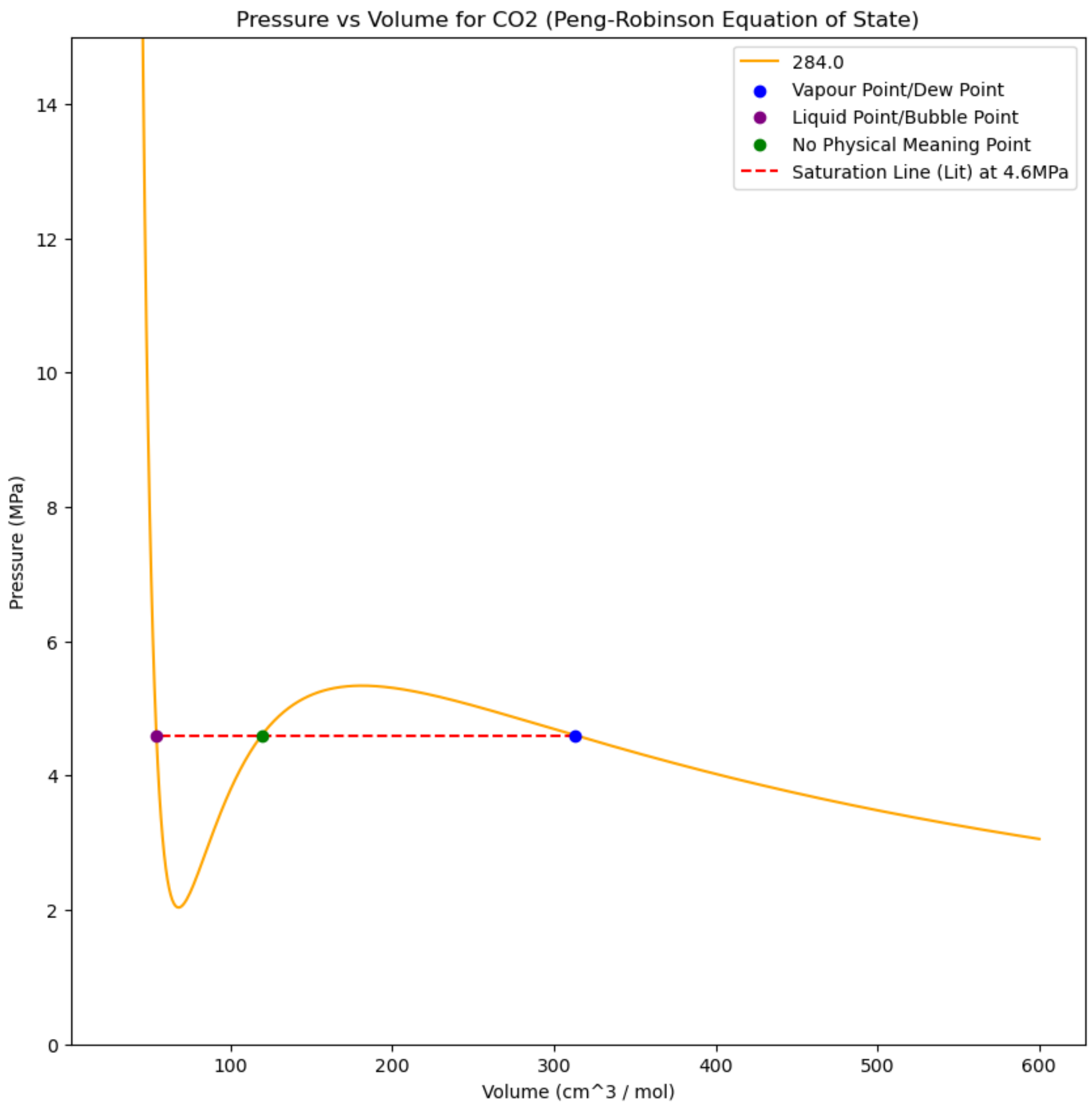
[51]:
```
Vc_root0 = Z_roots[0]* R * T / P
print(f' At Z = {Z_roots[0]}, the Volume is {Vc} cm^3/mol. This is the Vapour␣
 ↪phase (Plot on graph)')
```

```
At Z = 0.6101610560175712, the Volume is 119.25981783492531 cm^3/mol. This is
the Vapour phase (Plot on graph)
```

[52]:
```
Vc_root2 = Z_roots[2]* R * T / P
print(f' At Z = {Z_roots[2]}, the Volume is {Vc} cm^3/mol. There is no physical␣
↪meaning (Plot on graph)')
```

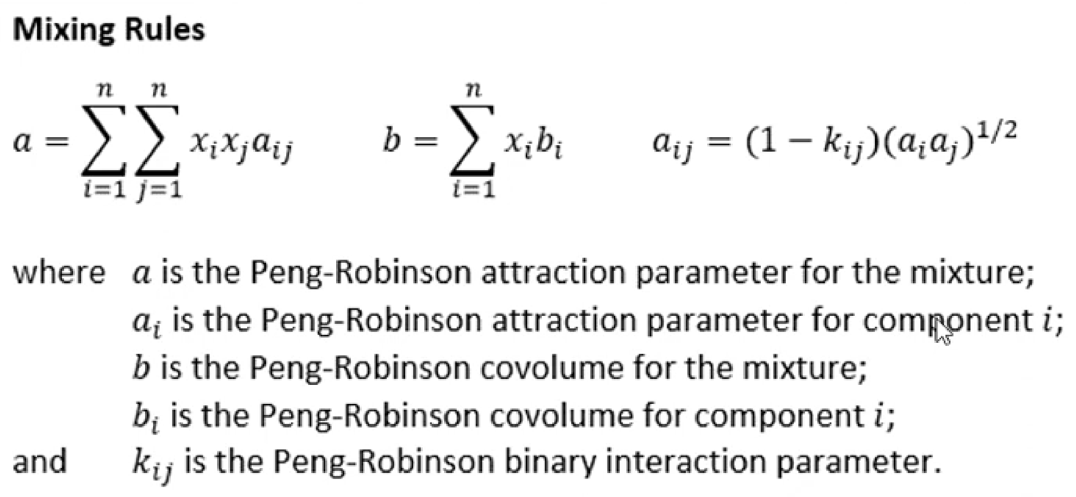
```
At Z = 0.2323398010316285, the Volume is 119.25981783492531 cm^3/mol. There is
no physical meaning (Plot on graph)
```

[67]:
```
# Plot preos_df, each column of the dataframe as a line on the same plot with␣
↪index as x-axis and pressure as y-axis, reduce y axis from 0 to 15
# Plot the critical point as a red dot
plt.figure(figsize = (10, 10))
for column in preos_df:
    if column == '284.0':
        plt.plot(preos_df.index, preos_df[column], label = column, color =␣
↪'orange')
plt.xlabel('Volume (cm^3 / mol)')
plt.ylabel('Pressure (MPa)')
plt.ylim(0, 15)
plt.title('Pressure vs Volume for CO2 (Peng-Robinson Equation of State)')

# plot the Z_roots and Vc on the same plot and the dot on top of the 284 line

plt.scatter(Vc_root0, P, color = 'blue', label = 'Vapour Point/Dew␣
↪Point',zorder=3)
plt.scatter(Vc_root1, P, color = 'purple', label = 'Liquid Point/Bubble Point',␣
↪zorder=3)
plt.scatter(Vc_root2, P, color = 'green', label = 'No Physical Meaning Point',␣
↪zorder=3)
#Draw a dotted line connecting the roots at P
plt.plot([Vc_root0, Vc_root1], [P, P], color = 'red', linestyle = '--', label =␣
↪'Saturation Line (Lit) at 4.6MPa', zorder=2)

plt.legend()
plt.show()
```


Pressure vs Volume for CO2 (Peng-Robinson Equation of State)
284.0
Vapour Point/Dew Point
Liquid Point/Bubble Point
No Physical Meaning Point
Saturation Line (Lit) at 4.6MPa
Pressure (MPa)
Volume (cm^3 / mol)
0
2
4
6
8
10
12
14
100
200
300
400
500
600

```
[ ]:
```

3 Mixing Rules



Mixing Rules

$$a = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j a_{ij} \qquad b = \sum_{i=1}^{n} x_i b_i \qquad a_{ij} = (1 - k_{ij})(a_i a_j)^{1/2}$$

where a is the Peng-Robinson attraction parameter for the mixture;
a_i is the Peng-Robinson attraction parameter for component i;
b is the Peng-Robinson covolume for the mixture;
b_i is the Peng-Robinson covolume for component i;
and k_{ij} is the Peng-Robinson binary interaction parameter.

[68]:
```
R = 8.314 # J/(mol*K)
T = 233.2 # K
P = 0.1 # MPa
```

[69]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

[79]:
```
df_data = pd.read_csv("./Critical_Constants_and_Acentric_Factors.csv")
```

[80]:
```
df_data
```

[80]:
```
                                Element   Tc(K)  Pc(bar)  Vc(cm3/mol)      w
0                                 Argon  150.80    48.70         74.9  0.001
1                               Bromine  588.00   103.00        127.2  0.108
2                              Chlorine  416.90    79.80        123.8  0.090
3                              Fluorine  144.30    52.20         66.3  0.054
4                              Helium-4    5.19     2.27         57.4 -0.365
..                                  …      …       …          …      …
71                           1-Propanol  536.80    51.70        219.0  0.623
72                             Pyridine  620.00    56.30        254.0  0.243
73   Trichlorotrifluoroethane (Freon 113)  487.30    34.10        325.5  0.256
74      Trichlorofluoromethane (Freon 11)  471.20    44.10        247.8  0.189
75                        Trimethylamine  433.30    40.90        254.0  0.205

[76 rows x 5 columns]
```

[72]:
```
molecules = ['Methane', 'Ethane', 'Propane']
```

[73]:
```
mol_fraction = [0.1, 0.3, 0.6]
```

[104]:
```
# Let's create a table where the molecules are the columns and the rows are the␣
↪mol_fraction, critical pressure, critical temperature, and acentric factor
df = pd.DataFrame(columns = molecules, index = ['Mol Fraction', 'Critical␣
↪Pressure (MPa)', 'Critical Temperature (K)', 'Acentric Factor', 'bi', 'ki',␣
↪'ai'])
df.loc['Mol Fraction'] = mol_fraction
#Critical Pressure and temperature from df_data using the molecules from the␣
↪column Element and pressure converting from bar to MPa
df.loc['Critical Pressure (MPa)'] = df_data.loc[df_data['Element'].
↪isin(molecules), 'Pc(bar)'].values * 0.1
df.loc['Critical Temperature (K)'] = df_data.loc[df_data['Element'].
↪isin(molecules), 'Tc(K)'].values
df.loc['Acentric Factor'] = df_data.loc[df_data['Element'].isin(molecules),␣
↪'w'].values

# Find bi for each molecule - 0.0778*R*Tc/Pc
df.loc['bi'] = 0.0778 * R * df.loc['Critical Temperature (K)'] / df.
↪loc['Critical Pressure (MPa)']
#Find ki for each molecule - 0.37464 + 1.54226*w - 0.26992*w**2
df.loc['ki'] = 0.37464 + 1.54226 * df.loc['Acentric Factor'] - 0.26992 * df.
↪loc['Acentric Factor']**2
#Find ai which involves alpha ai for each molecule - 0.45724*R**2*Tc**2/Pc * (1␣
↪+ ki(1 - (T/Tc)**0.5))**2
df.loc['ai'] = 0.45724 * R**2 * df.loc['Critical Temperature (K)']**2 / df.
↪loc['Critical Pressure (MPa)'] * (1 + df.loc['ki'] * (1 - (T/df.
↪loc['Critical Temperature (K)'])**0.5))**2
```

[105]:
```
df
```

[105]:
```
                                  Methane         Ethane         Propane
Mol Fraction                          0.1            0.3             0.6
Critical Pressure (MPa)              4.88            4.6            4.25
Critical Temperature (K)            305.4          190.4           369.8
Acentric Factor                     0.099          0.011           0.153
bi                              40.479844      26.773104        56.28175
ki                               0.524678       0.391572        0.604287
ai                          686683.081716  228701.643792  1285770.861809
```

3.1 Interactions Parameter

i, j	Methane	Ethane	Propane
Methane	0	0.00340	0.01070
Ethane	0.0340	0	0.00900

i, j	Methane	Ethane	Propane
Propane	0.0170	0.00900	0

[106]:
```
df_interaction = pd.DataFrame(columns = molecules, index = molecules)
df_interaction = df_interaction.fillna(0.0)
df_interaction = df_interaction.astype(float)
df_interaction.loc['Methane', 'Methane'] = 0.0
df_interaction.loc['Methane', 'Ethane'] = 0.00340
df_interaction.loc['Methane', 'Propane'] = 0.01070
df_interaction.loc['Ethane', 'Methane'] = 0.00340
df_interaction.loc['Ethane', 'Ethane'] = 0.0
df_interaction.loc['Ethane', 'Propane'] = 0.00900
df_interaction.loc['Propane', 'Methane'] = 0.01070
df_interaction.loc['Propane', 'Ethane'] = 0.00900
df_interaction.loc['Propane', 'Propane'] = 0.0
```

[107]:
```
df_interaction
```

[107]:
```
         Methane  Ethane  Propane
Methane   0.0000  0.0034   0.0107
Ethane    0.0034  0.0000   0.0090
Propane   0.0107  0.0090   0.0000
```

[108]:
```
# Create table of aij using the interaction table and the ai table
df_aij = pd.DataFrame(columns = molecules, index = molecules)
# Formulae for aij - sqrt(ai*aj)*(1 - kij)
for i in molecules:
    for j in molecules:
        df_aij.loc[i, j] = (df.loc['ai', i] * df.loc['ai', j])**0.5 * (1 -␣
 ↪df_interaction.loc[i, j])
df_aij
```

[108]:
```
               Methane         Ethane         Propane
Methane  686683.081716  394942.344225   929582.571402
Ethane   394942.344225  228701.643792   537390.626968
Propane  929582.571402  537390.626968  1285770.861809
```

[114]:
```
# Multiple the aij table by the mol_fraction table
df_aij_mol_fraction = pd.DataFrame(columns = molecules, index = molecules)
for i in molecules:
    for j in molecules:
        print (i, j)
        print (df_aij.loc[i, j])
        print (df.loc['Mol Fraction', i])
        print (df.loc['Mol Fraction', j])
        df_aij_mol_fraction.loc[i, j] = df_aij.loc[i, j] * df.loc['Mol␣
↪Fraction', i] * df.loc['Mol Fraction', j]
df_aij_mol_fraction
```

```
Methane Methane
686683.0817162682
0.1
0.1
Methane Ethane
394942.34422541014
0.1
0.3
Methane Propane
929582.5714019976
0.1
0.6
Ethane Methane
394942.34422541014
0.3
0.1
Ethane Ethane
228701.64379200127
0.3
0.3
Ethane Propane
537390.6269677967
0.3
0.6
Propane Methane
929582.5714019976
0.6
0.1
Propane Ethane
537390.6269677967
0.6
0.3
Propane Propane
1285770.861809112
0.6
0.6
```

[114]:

```
              Methane        Ethane        Propane
Methane   6866.830817  11848.270327   55774.954284
Ethane   11848.270327  20583.147941   96730.312854
Propane  55774.954284  96730.312854  462877.510251
```

[117]:
```
# Peng-Robinson Equation of State for a mixture of 3 components
# Sum all values in the aij_mol_fraction table and it will equal a(T)
a = df_aij_mol_fraction.sum().sum()
print(a)
```

```
819034.5639398942
```

[119]:
```
# Sum all values in the bi_mol_fraction table and it will equal b(T)
b = (df.loc['bi'] * df.loc['Mol Fraction']).sum()
print(b)
```

```
45.84896575534325
```

3.1.1 Cubic Equation

m(3) * Z^3 + m(2) * Z^2 + m(1) * Z + m(0) = 0

[121]:
```
# Find A and B
A = a * P / (R**2 * T**2)
B = b * P / (R * T)
print(A)
print(B)
```

```
0.021788387838798252
0.0023647812713837404
```

[127]:
```
# Find the Z_roots for the mixture
m3 = 1
```

[122]:
```
m2 = -1 - B
```

[123]:
```
m1 = A - 3 * B**2 - 2 * B
```

[125]:
```
m0 = -A * B + B**2 + B**3
```

[128]:
```
print( m3, m2, m1, m0)
```

```
1 -1.0023647812713838 0.017042048724646312 -4.591935672607873e-05
```

[129]:
```
Z_roots_mix = ces.solve(m3, m2, m1, m0)
```

[130]:
```
Z_roots_mix
```

[130]:
```
array([0.9851125 , 0.00335386, 0.01389842])
```

3.1.2 Finding the fugacity coefficient for all components

[139]:
```
# Create table of xi (mole fraction) and  df_aij where mol fraction * aij
df_xi = pd.DataFrame(columns = molecules, index = molecules)
for i in molecules:
    for j in molecules:
        print (i, j)
        print (df.loc['Mol Fraction', i])
        print (df_aij.loc[i, j])
        df_xi.loc[i, j] = df.loc['Mol Fraction', i] * df_aij.loc[i, j]
df_xi
```

```
Methane Methane
0.1
686683.0817162682
Methane Ethane
0.1
394942.34422541014
Methane Propane
0.1
929582.5714019976
Ethane Methane
0.3
394942.34422541014
Ethane Ethane
0.3
228701.64379200127
Ethane Propane
0.3
537390.6269677967
Propane Methane
0.6
929582.5714019976
Propane Ethane
0.6
537390.6269677967
Propane Propane
0.6
1285770.861809112
```

[139]:
```
               Methane         Ethane        Propane
Methane   68668.308172   39494.234423    92958.25714
Ethane   118482.703268   68610.493138   161217.18809
Propane  557749.542841  322434.376181  771462.517085
```

[171]:
```
# Sum each column in the df_xi table
df_xi.sum(axis = 0)
df_sum_xi = pd.DataFrame(columns = molecules, index = ['Sum_xi'])
```

```
df_sum_xi.loc['Sum_xi'] = df_xi.sum(axis = 0)
df_sum_xi
```

[171]:

```
              Methane         Ethane         Propane
Sum_xi  744900.55428  430539.103741  1025637.962316
```

[178]:

```
# Find the fugacity coefficients for each component at Z root mix 0 and 2
# Column is Z, methan_fug, ethane_fug, propane_fug
# Index is liq_phase, no_physical_meaning, vap_phase
df_fug = pd.DataFrame(columns = [str('Z')] + molecules, index = ['liq_phase',␣
 ↪'no_physical_meaning', 'vap_phase'])

# Column Z is the Z_roots_mix
df_fug.loc['liq_phase', 'Z'] = Z_roots_mix[1]
df_fug.loc['no_physical_meaning', 'Z'] = Z_roots_mix[2]
df_fug.loc['vap_phase', 'Z'] = Z_roots_mix[0]

# Fugacity coefficients for each component at Z root mix 0, using df_sum_xi and␣
 ↪df_aij
#
# Formulae for fugacity coefficients - exp(((bi/b)*(Z-1)) -(log(Z-B)) -(A/
 ↪(2*sqrt(2)*B))*(2*(df_sum_xi.loc['Sum xi', i])*df_aij.loc[i, i])/a) * LN((Z+␣
 ↪2.414*B)/(Z-0.414*B))
#

for i in molecules:
    # Let's break it up for liq_phase
    # First part of the equation
    first_part = (df.loc['bi', i] / b) * (1-df_fug.loc['liq_phase', 'Z'])
    print(first_part)
    # Second part of the equation
    second_part = np.log(df_fug.loc['liq_phase', 'Z'] - B)
    # Third part of the equation
    third_part_1 = A / (2 * 2**0.5 * B)
    third_part_2 = ((2 * df_sum_xi.loc['Sum_xi', i]/a)- (df.loc['bi', i]/b))
    third_part_3 = np.log((df_fug.loc['liq_phase', 'Z'] + 2.414 * B) / (df_fug.
 ↪loc['liq_phase', 'Z'] - 0.414 * B))
    third_part = third_part_1 * third_part_2 * third_part_3
    # Fugacity coefficient for liq_phase
    df_fug.loc['liq_phase', i] = np.exp(first_part - second_part - third_part)

    # For vap_phase
    # First part of the equation
    first_part = (df.loc['bi', i] / b) * (1-df_fug.loc['vap_phase', 'Z'])
    print(first_part)
    # Second part of the equation
    second_part = np.log(df_fug.loc['vap_phase', 'Z'] - B)
    # Third part of the equation
    third_part_1 = A / (2 * 2**0.5 * B)
    third_part_2 = ((2 * df_sum_xi.loc['Sum_xi', i]/a)- (df.loc['bi', i]/b))
    third_part_3 = np.log((df_fug.loc['vap_phase', 'Z'] + 2.414 * B) / (df_fug.
↪loc['vap_phase', 'Z'] - 0.414 * B))
    third_part = third_part_1 * third_part_2 * third_part_3
    # Fugacity coefficient for vap_phase
    df_fug.loc['vap_phase', i] = np.exp(first_part - second_part - third_part)
```

```
0.8799343570732929
0.013144103885122388
0.5819828362969195
0.008693424456215113
1.2234297617004004
0.01827509944881167
```

[179]:
```
df_fug
```

[179]:
```
                           Z    Methane     Ethane    Propane
liq_phase           0.003354  41.059377  235.50114  13.084299
no_physical_meaning 0.013898        NaN        NaN        NaN
vap_phase           0.985113   1.009945    1.01591   1.007535
```

[177]:
```
import preos
```

[ ]:
```

```