Homework Assignment Number Nine Solutions

Problem 1. (8 points)

Consider the Peng-Robinson Equation of state as given below. The critical temperature and pressure of oxygen are also given below. Each root of this equation is a molar volume. Find all of the roots of the Peng-Robinson equation for oxygen at the temperatures given below and for a pressure of 1.0 atmosphere.

(a) T = 98.0 K

(b) T = 298.0 K

(For those of you who have not had thermodynamics, there can only be one phase above the critical temperature.)

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)}$$

where, $R = 8.314$ J/mol/K, and $a(T) = 0.45724\frac{R^2{T_c}^2}{P_c}\alpha(T)$, $b = 0.07780\frac{RT_c}{P_c}$, $\alpha(T) = \left[1 + \kappa\left(1 - \sqrt{\frac{T}{T_c}}\right)\right]^2$ where, for the oxygen molecule $\kappa = 0.4069$, $T_c = 154.6$ K, and $P_c = 5.046 \cdot 10^6$ Pa.

Solution:

Solution in Python:

Using the Newton-Raphson method with numerical derivatives as implemented in the code, nrnd1.py, we input the function,

```
def funkeval(x):
    V = x # molar volume is unknown
    T = 98.0 # K
    p = 101325.0 # Pa
    R = 8.314 # J/mol/K
    Tc = 154.6 # K
    pc = 5.046e+6 # Pa
    kappa = 0.4069
    alpha = (1.0 + kappa*(1.0 - np.sqrt(T/Tc)))**2
    b = 0.07780*R*Tc/pc
    a = 0.45724*R**2*Tc**2/pc*alpha
    f = R*T/(V-b) - a/(V*(V+b) + b*(V-b)) - p;
    return f
```

(a) T = 98.0 K

This temperature is below the critical temperature. We should find three roots. We wrote a script to solve for all three roots. In the script below, we call nrnd1.py three times. Each time we feed the function a different initial guess. To find the gas molar volume, we used the ideal gas law as an initial guess. To find the liquid root, we used an initial guess 10% larger than the b parameter. To find the middle root, we used an initial guess 10 times larger than the b parameter

```
import numpy as np
from nrnd1_hw09_p01 import *

# Problem 1
# Part (a) T = 98 K

T = 98.0 # K

p = 101325.0 # Pa
R = 8.314 # J/mol/K
Tc = 154.6 # K
```

```
pc = 5.046e+6 # Pa
kappa = 0.4069
alpha = (1.0 + kappa*(1.0 - np.sqrt(T/Tc)))**2
b = 0.07780*R*Tc/pc
a = 0.45724*R**2*Tc**2/pc*alpha

# initial guess for gas root using ideal gas law
Vig_gas = R*T/p
Vgas, error = nrnd1(Vig_gas)
print(f"molar volume of gas = {Vgas} m^3/mol")

# initial guess for liquid root (10% bigger than b)
Vig_liq = 1.1*b
Vliq, error = nrnd1(Vig_liq)
print(f"molar volume of liquid = {Vliq} m^3/mol")

# initial guess for middle root (10 times bigger than b)
Vig_mid = 10.0*b
Vmid, error = nrnd1(Vig_mid)
print(f"molar volume of middle root = {Vmid} m^3/mol")
```

Running this script yielded the following results.

```
run hw09_p01.py
icount = 1, xold = 8.041174e-03, f = -2.451572e+03, df = -1.199388e+07, xnew = 7.836772e-03, err = 1.000000e+02
icount = 2, xold = 7.836772e-03, f = 6.205521e+01, df = -1.261114e+07, xnew = 7.841693e-03, err = 6.275005e-04
icount = 3, xold = 7.841693e-03, f = 4.381760e-02, df = -1.259573e+07, xnew = 7.841697e-03, err = 4.436243e-07
molar volume of gas = 0.007841696625974268 m^3/mol
icount = 1, xold = 2.179940e-05, f = 2.255431e+08, df = -1.936839e+14, xnew = 2.296389e-05, err = 1.000000e+02
icount = 2, xold = 2.296389e-05, f = 9.082289e+07, df = -6.898469e+13, xnew = 2.428046e-05, err = 5.422328e-02
icount = 3, xold = 2.428046e-05, f = 3.100786e+07, df = -2.950358e+13, xnew = 2.533144e-05, err = 4.148940e-02
icount = 4, xold = 2.533144e-05, f = 7.546792e+06, df = -1.675601e+13, xnew = 2.578184e-05, err = 1.746939e-02
icount = 5, xold = 2.578184e-05, f = 8.142871e+05, df = -1.338101e+13, xnew = 2.584269e-05, err = 2.354783e-03
icount = 6, xold = 2.584269e-05, f = 1.445433e+04, df = -1.298809e+13, xnew = 2.584380e-05, err = 4.306218e-05
icount = 7, xold = 2.584380e-05, f = 4.755343e+01, df = -1.298103e+13, xnew = 2.584381e-05, err = 1.417477e-07
molar volume of liquid = 2.584380714495502e-05 m^3/mol
icount = 1, xold = 1.981764e-04, f = 7.102706e+05, df = 9.434822e+09, xnew = 1.228945e-04, err = 1.000000e+02
icount = 2, xold = 1.228945e-04, f = -1.162861e+06, df = 5.401781e+10, xnew = 1.444219e-04, err = 1.490588e-01
icount = 3, xold = 1.444219e-04, f = -2.662415e+05, df = 3.161276e+10, xnew = 1.528439e-04, err = 5.510174e-02
icount = 4, xold = 1.528439e-04, f = -2.491949e+04, df = 2.592112e+10, xnew = 1.538052e-04, err = 6.250493e-03
icount = 5, xold = 1.538052e-04, f = -2.822961e+02, df = 2.534838e+10, xnew = 1.538164e-04, err = 7.240226e-05
icount = 6, xold = 1.538164e-04, f = -1.036041e-01, df = 2.534183e+10, xnew = 1.538164e-04, err = 2.657887e-08
molar volume of middle root = 0.00015381636861737315 m^3/mol
```

Therefore, the vapor root is 0.00784 m^3/mole.
The liquid root is 2.58×10^{-5} m^3/mole.
The intermediate root is 1.54×10^{-4} m^3/mole.

(b) T = 298.0 K

This temperature is above the critical temperature. We should find one root.

First, I change the input function in nrnd1.m. The only change is a change in temperature.

```
def funkeval(x):
    V = x # molar volume is unknown
    T = 298.0 # K
    p = 101325.0 # Pa
    R = 8.314 # J/mol/K
    Tc = 154.6 # K
    pc = 5.046e+6 # Pa
    kappa = 0.4069
    alpha = (1.0 + kappa*(1.0 - np.sqrt(T/Tc)))**2
    b = 0.07780*R*Tc/pc
    a = 0.45724*R**2*Tc**2/pc*alpha
```

```
    f = R*T/(V-b) - a/(V*(V+b) + b*(V-b)) - p;
    return f
```

I used the same cript as for part (a) but changed the temperature. I still assumed that the ideal gas should give a good estimate of the root.

```
import numpy as np
from nrnd1_hw09_p01b import *

# Problem 1
# Part (b) T = 298 K

T = 298.0 # K
p = 101325.0 # Pa
R = 8.314 # J/mol/K
Tc = 154.6 # K
pc = 5.046e+6 # Pa
kappa = 0.4069
alpha = (1.0 + kappa*(1.0 - np.sqrt(T/Tc)))**2
b = 0.07780*R*Tc/pc
a = 0.45724*R**2*Tc**2/pc*alpha

# initial guess for gas root using ideal gas law
Vig_gas = R*T/p
Vgas, error = nrnd1(Vig_gas)
print(f"molar volume of gas = {Vgas} m^3/mol")
```

Running the script generated the following output.

```
run hw09_p01b.py
icount = 1, xold = 2.445173e-02, f = -9.503104e+01, df = -4.136532e+06, xnew = 2.442876e-02, err = 1.000000e+02
icount = 2, xold = 2.442876e-02, f = 7.979252e-02, df = -4.144309e+06, xnew = 2.442878e-02, err = 7.881489e-07
molar volume of gas = 0.02442878017087713 m^3/mol
```

Therefore, the root is 0.0244 m^3/mol.

Solution in Matlab:

Using the Newton-Raphson method with numerical derivatives as implemented in the code, nrnd1.m, we input the function,

```
function f = funkeval(x)
V = x;
T = 98; % K
p = 101325; % Pa
R = 8.314; % J/mol/K
Tc = 154.6; % K
pc = 5.046e+6; % Pa
kappa = 0.4069;
alpha = (1 + kappa*(1 - sqrt(T/Tc)))^2;
b = 0.07780*R*Tc/pc;
a = 0.45724*R^2*Tc^2/pc*alpha;
f = R*T/(V-b) - a/(V*(V+b) + b*(V-b)) - p;
```

(a) T = 98.0 K

This temperature is below the critical temperature. We should find three roots.

The ideal gas should give a good estimate of the vapor root

```
T = 98; % K
p = 101325; % Pa
R = 8.314; % J/mol/K
V = R*T/p

V =    0.008041174438687
```

We now run the Newton Raphson with Numerical Derivatives code for 1 unknown (nrnd1) with that initial guess.

```
>>  [x0,err] = nrnd1(0.008)
icount = 1 xold = 8.000000e-03 f = -1.955300e+03 df = -1.211452e+07 xnew = 7.838599e-03  err = 1.000000e+02
icount = 2 xold = 7.838599e-03 f = 3.903320e+01 df = -1.260542e+07 xnew = 7.841695e-03  err = 3.948818e-04
icount = 3 xold = 7.841695e-03 f = 1.871688e-02 df = -1.259572e+07 xnew = 7.841697e-03  err = 1.894962e-07

x0 =   0.007841696626165

err =     1.894961977606645e-07
```

Therefore, the vapor root is 0.00784 moles/m^3.

Next, we find the liquid root, which is a little larger, say 10% larger, than the b parameter. First we calculate b.

```
>> R = 8.314; % J/mol/K
Tc = 154.6; % K
pc = 5.046e+6; % Pa
b = 0.07780*R*Tc/pc

b =    1.981763660721363e-05
```

Then we run nrnd1 with a guess 10% larger than b.

```
>>  [x0,err] = nrnd1(1.1*1.98e-05)

icount = 1 xold = 2.178000e-05 f = 2.292908e+08 df = -1.978558e+14 xnew = 2.293888e-05  err = 1.000000e+02
icount = 2 xold = 2.293888e-05 f = 9.255337e+07 df = -7.027407e+13 xnew = 2.425591e-05  err = 5.429746e-02
icount = 3 xold = 2.425591e-05 f = 3.173420e+07 df = -2.992303e+13 xnew = 2.531644e-05  err = 4.189086e-02
icount = 4 xold = 2.531644e-05 f = 7.798334e+06 df = -1.688450e+13 xnew = 2.577830e-05  err = 1.791675e-02
icount = 5 xold = 2.577830e-05 f = 8.614611e+05 df = -1.340424e+13 xnew = 2.584257e-05  err = 2.486897e-03
icount = 6 xold = 2.584257e-05 f = 1.599850e+04 df = -1.298885e+13 xnew = 2.584380e-05  err = 4.765980e-05
icount = 7 xold = 2.584380e-05 f = 5.309695e+01 df = -1.298103e+13 xnew = 2.584381e-05  err = 1.582719e-07

x0 =    2.584380714366121e-05

err =    1.582718742543172e-07
```

Therefore, the liquid root is 2.58x10^{-5} moles/m^3.

Next we find the intermediate root. This root must be between the liquid and vapor root. We can try 10*b.

```
>>  [x0,err] = nrnd1(10*1.98e-05)

icount = 1 xold = 1.980000e-04 f = 7.086039e+05 df = 9.471210e+09 xnew = 1.231834e-04  err = 1.000000e+02
icount = 2 xold = 1.231834e-04 f = -1.147320e+06 df = 5.361335e+10 xnew = 1.445833e-04  err = 1.480109e-01
icount = 3 xold = 1.445833e-04 f = -2.611509e+05 df = 3.149117e+10 xnew = 1.528761e-04  err = 5.424543e-02
icount = 4 xold = 1.528761e-04 f = -2.408423e+04 df = 2.590168e+10 xnew = 1.538059e-04  err = 6.045494e-03
icount = 5 xold = 1.538059e-04 f = -2.641220e+02 df = 2.534796e+10 xnew = 1.538164e-04  err = 6.774216e-05
icount = 6 xold = 1.538164e-04 f = -9.473805e-02 df = 2.534183e+10 xnew = 1.538164e-04  err = 2.430434e-08

x0 =   1.538163686174564e-04

err =     2.430434345736832e-08
```

Therefore, the intermediate root is 1.54x10^{-4} moles/m^3.

(b) T = 298.0 K

This temperature is above the critical temperature. We should find one real root.

First, I change the input function in nrnd1.m. The only change is a change in temperature.

```
function f = funkeval(x)
V = x;
T = 298; % K
p = 101325; % Pa
R = 8.314; % J/mol/K
Tc = 154.6; % K
pc = 5.046e+6; % Pa
kappa = 0.4069;
alpha = (1 + kappa*(1 - sqrt(T/Tc)))^2;
b = 0.07780*R*Tc/pc;
a = 0.45724*R^2*Tc^2/pc*alpha;
f = R*T/(V-b) - a/(V*(V+b) + b*(V-b)) - p;
```

The ideal gas should give a good estimate of the root.

```
>> T = 298; % K
p = 101325; % Pa
R = 8.314; % J/mol/K
V = R*T/p

V =   0.024451734517641

>> [x0,err] = nrnd1(0.024)
icount = 1 xold = 2.400000e-02 f = 1.808531e+03 df = -4.293565e+06 xnew = 2.442122e-02  err = 1.000000e+02
icount = 2 xold = 2.442122e-02 f = 3.134197e+01 df = -4.146867e+06 xnew = 2.442878e-02  err = 3.093887e-04
icount = 3 xold = 2.442878e-02 f = 1.281518e-02 df = -4.144303e+06 xnew = 2.442878e-02  err = 1.265819e-07

x0 =   0.024428780172505

err =     1.265818784914305e-07
```

Therefore, the root is 0.0244 moles/m^3.

Problem 2. (6 points)

Consider the van der Waals equation of state. Vapor-liquid equilibrium at a given temperature, T, occurs at a specific pressure, the vapor pressure, p_{vap}. Therefore, we can consider the vapor pressure our unknown. However, you can't calculate the vapor pressure without knowing the molar volumes of the vapor, V_{vap}, and liquid, V_{liq}, phases. Therefore, we have three unknowns: p_{vap}, V_{vap} and V_{liq}. Solving a system of three equations and three unknowns is much harder than solving a system of equations with one equation and one unknown. Therefore, a useful trick in this problem is to recognize that the van der Waal's equation of state is a cubic equation of state and the roots of a cubic equation of state are easily obtained using the Matlab "roots" function. Therefore, we can pose the solution of the vapor-liquid equilibrium problem of the van der Waals fluid as a single equation with a single equation, in which we guess the vapor pressure, use the roots command to solve for the V_{vap} and V_{liq}. and substitute them into the equation stating that the chemical potentials are equal.

For your reference, the pressure of the van der Waal's equation of state is

$$p = \frac{RT}{V-b} - \frac{a}{V^2}$$

This is a cubic equation of state and can also be written as

$$pV^3 - (pb + RT)V^2 + aV - ab = 0$$

The chemical potential for a van der Waals gas is

$$\mu = -RT\left[ln\left(\frac{V\ -b}{\Lambda^3}\right) - \frac{b}{V-b} + \frac{2a}{VRT}\right]$$

This expression for the chemical potential of a van der Waals gas introduces a new constant, the thermal de Broglie wavelength, Λ, but we don't need it because it drops out when we equate chemical potentials.

$$\mu_{liq} - \mu_{vap} = -RT\left[ln\left(\frac{V_{liq}-b}{\Lambda^3}\right) - \frac{b}{V_{liq}-b} + \frac{2a}{V_{liq}RT}\right] + RT\left[ln\left(\frac{V_{vap}-b}{\Lambda^3}\right) - \frac{b}{V_{vap}-b} + \frac{2a}{V_{vap}RT}\right]$$
$$= -RT\left[ln\left(V_{liq}-b\right) - \frac{b}{V_{liq}-b} + \frac{2a}{V_{liq}RT}\right] + RT\left[ln\left(V_{vap}-b\right) - \frac{b}{V_{vap}-b} + \frac{2a}{V_{vap}RT}\right]$$

So, in order to solve this problem as a single nonlinear algebraic equation with a single variable, p_{vap}, we have an equation,

$$f\left(p_{vap}\right) = \mu_{liq} - \mu_{vap} = 0$$

where we solve for the molar volumes each iteration.

(a) Find the vapor pressure of Argon at T=77 K. The van der Waals constants for argon are a=0.1381 m^6/mol^2 and b=3.184x10^{-5} m^3/mol. The gas constant is R=8.314 J/mol/K.
(b) & (c) Also report the liquid and vapor molar volumes.

Solution:
Solution in Python:
First we modify the input function in nrnd1.py

```
def funkeval(x):
    p = x # Pa
    T = 77.0 # K
    R = 8.314 # J/mol/K
    a = 0.1381
    b = 3.184e-5
    Vvec = np.roots([p,-(p*b+R*T),a,-a*b])
    Vvap = max(Vvec)
    Vliq = min(Vvec)
    muliq = R*T*(np.log(Vliq-b) - b/(Vliq-b) + 2.0*a/(Vliq*R*T))
    muvap = R*T*(np.log(Vvap-b) - b/(Vvap-b) + 2.0*a/(Vvap*R*T))
    f = muliq - muvap
    return f
```

We can call nrnd1.py with a short script. We will guess that the vapor pressure is 10 bar (1013250 Pa).

```
import numpy as np
from nrnd1_hw09_p02 import *

# Problem 2
# Part (a) find vapor pressure

# initial guess
pig = 1013250.0 # Pa

pvap, error = nrnd1(pig)
print(f"vapor pressure = {pvap} Pa")
```

Running the script yielded:

```
run hw09_p02.py
icount = 1, xold = 1.013250e+06, f = 1.031053e+03+1.082254e+01j, df = 2.737566e-04+1.202749e-04j, xnew = -
2.158243e+06+1.353862e+06j, err = 1.000000e+02
icount = 2, xold = -2.158243e+06+1.353862e+06j, f = -1.728977e+03-1.315617e+03j, df = 4.561209e-04+1.679740e-04j, xnew =
2.115039e+06+2.664517e+06j, err = 1.313895e+00
icount = 3, xold = 2.115039e+06+2.664517e+06j, f = -9.449844e+02+5.438578e+02j, df = 1.105452e-04+3.252880e-04j, xnew =
1.501251e+06-4.491419e+05j, err = 2.025260e+00
...
icount = 100, xold = 1.218105e+06-9.865234e+05j, f = 9.694778e+02-2.055460e+02j, df = 1.291865e-04-9.308506e-05j, xnew = -
4.476334e+06-3.498560e+06j, err = 1.095501e+00
icount = 101, xold = -4.476334e+06-3.498560e+06j, f = -2.823699e+03+8.829421e+02j, df = 2.798239e-04-1.116730e-04j, xnew =
5.314533e+06-2.746539e+06j, err = 1.641464e+00
Sorry. You did not converge in 100 iterations.
The final value of x was 5.314533e+06-2.746539e+06j
vapor pressure = (5314532.858742742-2746539.483961149j) Pa)
```

The initial guess of 10 bar was a bad guess. It resulted in a complex result and did not converge in 100 iterations.. Let's rerun the same script with a new guess of 1 bar (101325 Pa).

```
icount = 1, xold = 1.013250e+05, f = -1.836244e+02, df = 6.089856e-03, xnew = 1.314775e+05, err = 1.000000e+02
icount = 2, xold = 1.314775e+05, f = -2.376403e+01, df = 4.639124e-03, xnew = 1.366000e+05, err = 3.750017e-02
icount = 3, xold = 1.366000e+05, f = -4.744128e-01, df = 4.456224e-03, xnew = 1.367065e+05, err = 7.787538e-04
icount = 4, xold = 1.367065e+05, f = -1.946897e-04, df = 4.452568e-03, xnew = 1.367065e+05, err = 3.198476e-07
vapor pressure = 136706.53798055937 Pa
```

Well, 1 bar was a good guess and converged. The vapor pressure of vdW Argon at 77 K is 1.367×10^5 Pa.

(b) & (c) Also report the liquid and vapor molar volumes.

To find the molar volumes, we can append a bit of code to the end of the script

```
import numpy as np
from nrnd1_hw09_p02 import *

# Problem 2
# Part (a) find vapor pressure

# a initial guess
pig = 101325.0 # Pa

pvap, error = nrnd1(pig)
print(f"vapor pressure = {pvap} Pa")

# part b
# determine molar volumes
p = pvap # Pa
T = 77.0 # K
R = 8.314 # J/mol/K
a = 0.1381
b = 3.184e-5
Vvec = np.roots([p,-(p*b+R*T),a,-a*b])
Vvap = max(Vvec)
Vliq = min(Vvec)
print(f"vapor molar volume = {Vvap} m^3/mol")
print(f"liquid molar volume = {Vliq} m^3/mol")
```

When we run the script, the following output is generated.

```
icount = 1, xold = 1.013250e+05, f = -1.836244e+02, df = 6.089856e-03, xnew = 1.314775e+05, err = 1.000000e+02
icount = 2, xold = 1.314775e+05, f = -2.376403e+01, df = 4.639124e-03, xnew = 1.366000e+05, err = 3.750017e-02
icount = 3, xold = 1.366000e+05, f = -4.744128e-01, df = 4.456224e-03, xnew = 1.367065e+05, err = 7.787538e-04
icount = 4, xold = 1.367065e+05, f = -1.946897e-04, df = 4.452568e-03, xnew = 1.367065e+05, err = 3.198476e-07
vapor pressure = 136706.53798055937 Pa
vapor molar volume = 0.004491379329434947 m^3/mol
liquid molar volume = 3.88128664780742e-05 m^3/mol
```

Therefore, the vapor root is 0.00449 m^3/mol and the liquid root is 3.88×10^{-5} m^3/mol.

Solution in Matlab:

First we modify the input function in nrnd1.m

```
function f = funkeval(x)
p = x;
T = 77; % K
R = 8.314; % J/mol/K
a = 0.1381;
b = 3.184e-5;
Vvec = roots([p,-(p*b+R*T),a,-a*b]);
Vvap = max(Vvec);
Vliq = min(Vvec);
muliq = R*T*(log(Vliq-b) - b/(Vliq-b) + 2*a/(Vliq*R*T));
muvap = R*T*(log(Vvap-b) - b/(Vvap-b) + 2*a/(Vvap*R*T));
f = muliq - muvap;
```

Next we guess that the vapor pressure is 10 atm (1013250 Pa).

```
>> [x0,err] = nrnd1(1013250)
icount = 1 xold = 1.013250e+06 f = 1.031053e+03 df = 2.737563e-04 xnew = -2.158245e+06  err = 1.000000e+02
...
icount = 100 xold = 1.808793e+07 f = 3.215774e+03 df = -6.053046e-05 xnew = 1.808841e+07  err =
1.650221e+00
icount = 101 xold = 1.808841e+07 f = 3.215771e+03 df = -6.052910e-05 xnew = 1.808742e+07  err =
1.650262e+00
Sorry.  You did not converge in 100 iterations.
The final value of x was 1.808742e+07

x0 =      1.808741850893457e+07 - 2.641805411122832e+07i

err =   1.650261686195342
```

Well, 10 atm was a bad guess and did not converge. Let's try a new guess of 1 atm (101325 Pa).

```
>> [x0,err] = nrnd1(101325)
icount = 1 xold = 1.013250e+05 f = -1.836244e+02 df = 6.089856e-03 xnew = 1.314775e+05  err = 1.000000e+02
icount = 2 xold = 1.314775e+05 f = -2.376403e+01 df = 4.639125e-03 xnew = 1.366000e+05  err = 3.750018e-02
icount = 3 xold = 1.366000e+05 f = -4.744139e-01 df = 4.456224e-03 xnew = 1.367065e+05  err = 7.787557e-04
icount = 4 xold = 1.367065e+05 f = -1.946510e-04 df = 4.452568e-03 xnew = 1.367065e+05  err = 3.197840e-07

x0 =     1.367065379805641e+05

err = 3.197840381851619e-07
```

Well, 1 atm was a good guess and converged. The vapor pressure of vdW Argon at 77 K is 1.367×10^5 Pa.

The corresponding liquid and vapor molar volumes are

```
>> p = x0

p =      1.367065379805641e+05

>> T = 77; % K
R = 8.314; % J/mol/K
a = 0.1381;
b = 3.184e-5;
Vvec = roots([p,-(p*b+R*T),a,-a*b]);
Vvap = max(Vvec)
Vliq = min(Vvec)

Vvap =    0.004491379329435

Vliq =      3.881286647807421e-05
```

Therefore, the vapor root is 0.00449 moles/m^3 and the liquid root is 3.88x10-5 moles/m^3.