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EQUATIONS OF STATE IN CHEMICAL ENGINNERING USING PYTHON

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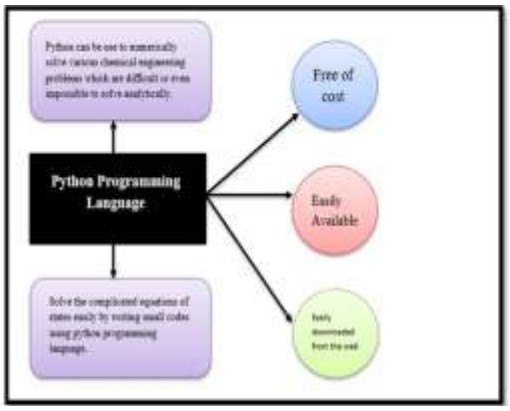
Abstract- **The python programming language is very useful for all kinds of scientific and engineering tasks by plotting data and analyzing various problems as well. We can use google Colab for python to numerically solve various chemical engineering problems which are difficult or even impossible to solve analytically. One of the best advantages of python programming language is that it is free of cost, and can be easily downloaded from the web.**
Solving equations of state allows us to find the specific volume of a gaseous mixture of various chemicals at a specified temperature and pressure. Without using the equation of state, it would be difficult for us to design a chemical plant virtually. By knowing the specific volume, we can determine the size and cost of the chemical plant, including the diameter of pipes, distillation towers and chemical reactors, the horsepower of compressors and pumps. This paper illustrates how to solve the complicated equations of states easily by writing small codes using python programming language.

Keywords: **Python programming language, Google Colab, Specific Volumes of gaseous mixture.**

Graphical Abstract


Python can be use to numerically solve various chemical engineering problems which are difficult or even impossible to solve analytically.
Python Programming Language
Solve the complicated equations of states easily by writing small codes using python programming language.
Free of cost
Easily Available
Easily downloaded from the web

I. INTRODUCTION

MATHEMATICAL STATEMENT OF EQUATIONS OF STATE

The ideal gas equation of state, which relates the Pressure, Specific Volume and Temperature is given by following formula:

$$pV = nRT \quad \text{or} \quad p\hat{v} = RT \quad \text{where } \hat{v} = \frac{V}{n} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.1)$$

The term p is absolute pressure, V is volume, n is the number of moles, R is the universal gas constant, T is the absolute temperature, and is the specific volume.

Also, the generalized formula of the ideal gas law was the van der waals equation of state which is given by the following formula:

$$p = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.2)$$

Here, "a" is the interaction force between two molecules and "b" is the excluded volume which means a second molecule cannot use the same space already used by the first molecule. Since the above van der waals equation is not a good approximation at high pressures therefore we define Redlich -Kwong equation of state which is the modification of van der waals equation of state given by the following formula:

$$p=\frac{RT}{\hat{v}-b}-\frac{a}{\hat{v}(\hat{v}+b)} \;\ldots\ldots\ldots\ldots\ldots (1.3)$$

Where,

$$a=0.42748\left(\frac{R^2T_c^2}{p_c}\right)\alpha\ ,\ b=0.08664\left(\frac{RT_c}{p_c}\right)\ ,\ \text{and}\ T_r=\frac{T}{T_c},\alpha=\frac{1}{T_r^{0.5}} \;\ldots\ldots\ldots\ldots\ldots (1.4)$$

Here, T_C is the critical temperature, p_C is the critical pressure, T_r is the reduced temperature which is the absolute temperature per critical temperature, and α is the particular to the Redlich -Kwongequation of state.[1]

Similarly, Redlich-kwong -soave equation of state is introduced which is the modified version of Redlich-kwong equation of state which is given by the following equation:

$$p=\frac{RT}{\hat{v}-b}-\frac{a}{\hat{v}(\hat{v}+b)} \;\ldots\ldots\ldots\ldots\ldots (1.5)$$

Now the term α is given by a different formula,

$$\alpha=[1+m(1-T_r^{0.5})]^2,\ \ m=0.480+1.574\omega+0.176\omega^2 \;\ldots\ldots\ldots\ldots\ldots (1.6)$$

Here the term □ is the acentric factor which is tabulated quantity for different substances. Therefore, the value of □ can be performed for each chemical and reduced temperature.

Peng-Robinson equation, which is another variation of equation of states and is given by thefollowing equation:

$$p=\frac{RT}{\hat{v}-b}-\frac{a}{\hat{v}(\hat{v}+b)+b(\hat{v}-b)} \;\ldots\ldots\ldots\ldots\ldots (1.7)$$

All of the above equations can be rearranged into a cubic function of specific volume and is given by the following equation:

$$\hat{v}^3(p)-\hat{v}^2(RT)+\hat{v}(a-pb^2-RTb)-ab=0 \;\ldots\ldots\ldots\ldots\ldots (1.8)$$

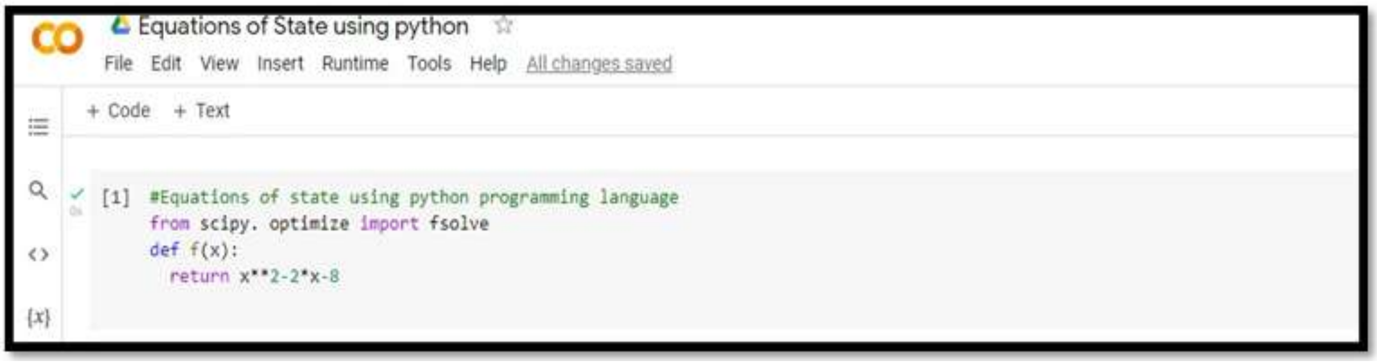
II. SOLVING EQUATIONS OF STATE USING PYTHON PROGRAMMING LANGUAGE (SINGLE EQUATION IN ONE UNKNOWN)

Nonlinear algebraic equations like equation of state can be solved using Python, too. First, we haveto define the problem statement to solve by defining a function; then, we check it; finally, we issue a command along with correct syntax to solve it.[2]

For example, we take the following equation and solve this with the help of python programminglanguage

$$f(x)=x^2-2x-8$$

There are various simple steps which we have to remember while solving the problem statement. Step 1: Firstly, Import the fsolve program from SciPy and define the function.


Equations of State using python
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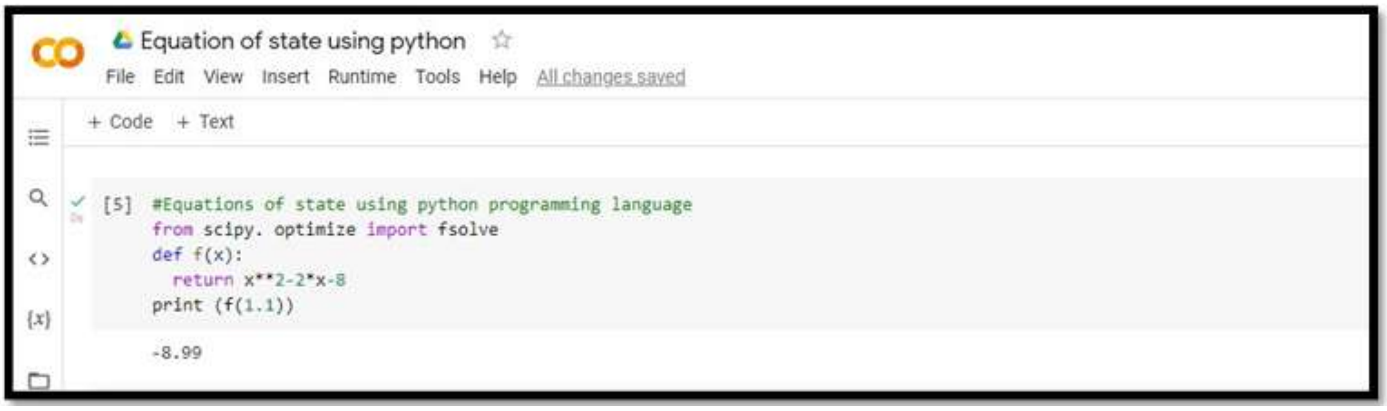
[1]

```
#Equations of state using python programming language
from scipy. optimize import fsolve
def f(x):
  return x**2-2*x-8
```

Figure 1: Import the fsolve program.

NOTE: The indentation after the declaration def f(x) which is mandatory in python to define theblocks of statements.
Step 2: Now, Check the function and issue a command in which we find the value of function atx=1.1 and we get the required result i.e., -8.99 that means the function f(x) is correct.


Equation of state using python
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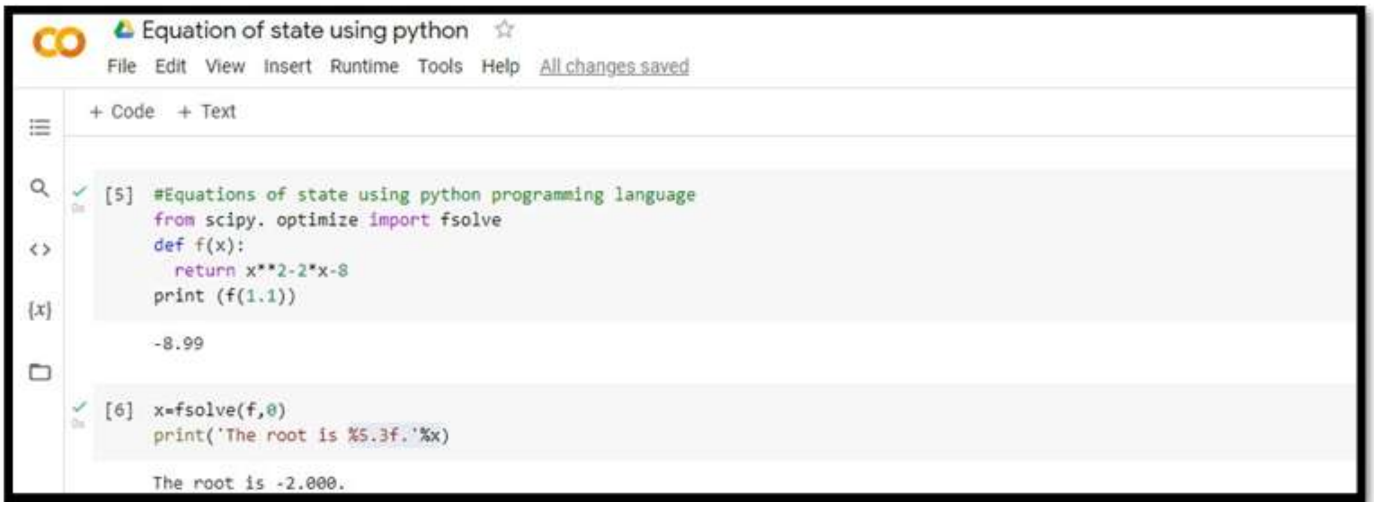
```
[5] #Equations of state using python programming language
    from scipy. optimize import fsolve
    def f(x):
      return x**2-2*x-8
    print (f(1.1))

    -8.99
```

Figure 2: Check the function and issue a command.

NOTE: In the above code we used a value of "x" that means every term in the function was important.
Step 3: We use the f solve function in python to find the value of x that makes the function i.e., f(x)=0.


Equation of state using python
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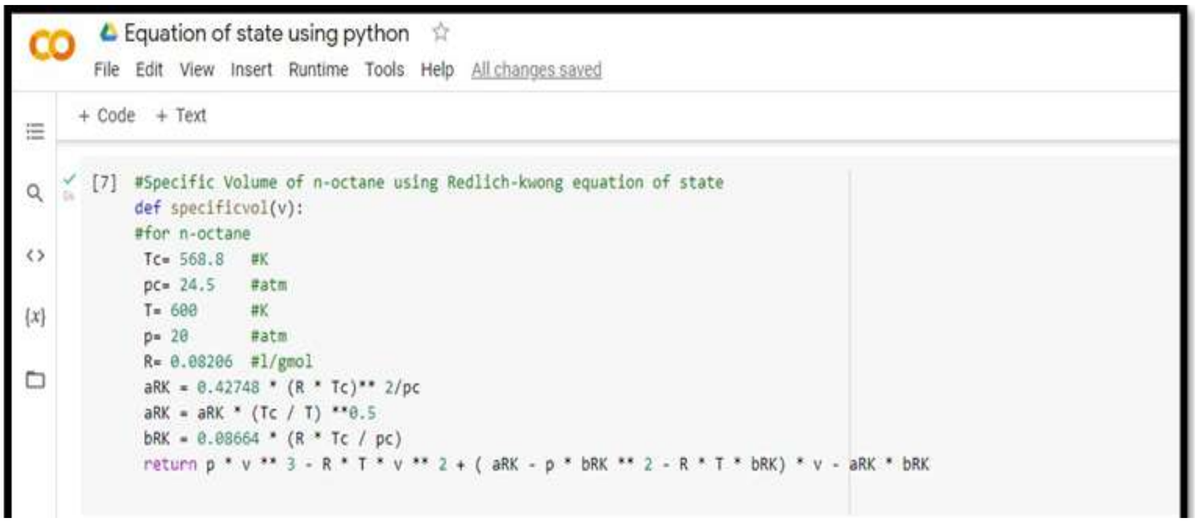
```
[5] #Equations of state using python programming language
    from scipy. optimize import fsolve
    def f(x):
      return x**2-2*x-8
    print (f(1.1))

    -8.99

[6] x=fsolve(f,0)
    print('The root is %5.3f.'%x)

    The root is -2.000.
```

Figure 3: Find the values of "x".

Here, %5.3f will mean that the width of the floating-point number should be 5.3. This command solves the following problem for x: f(x) = 0 starting from the initial guess of 0 and we get the required result i.e., -2.000.
To summarize the steps, In Step 1 we defined the problem we wish to solve using python and evaluated the problem for some "x", Step 2 we check the function and issue a command to find the value of the function and in Step 3 we instructed python to solve the problem. Hence the problem become easier by applying all the correct syntax and commands in python programminglanguage.[3]

Examples of solving Chemical Engineering Problems with the help of PythonProgramming Language

Example 1: Find the specific volume of n-octane at 600°K and 20 atm using the Redlich-Kwongequation of state.
Step 1: Firstly, define the function that will calculate the f(x), here specificvol (v), given the temperature, pressure, and thermodynamic properties.


Equation of state using python
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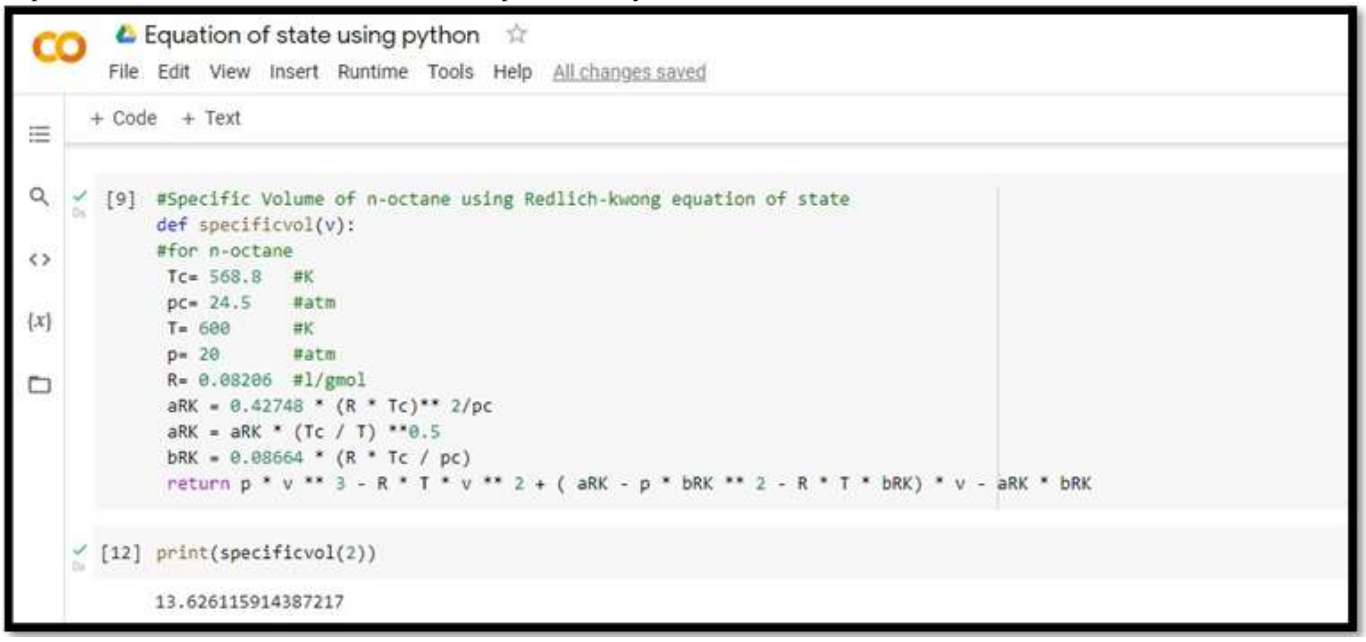
```
[7] #Specific Volume of n-octane using Redlich-kwong equation of state
    def specificvol(v):
    #for n-octane
     Tc= 568.8   #K
     pc= 24.5    #atm
     T= 600      #K
     p= 20       #atm
     R= 0.08206  #l/gmol
     aRK = 0.42748 * (R * Tc)** 2/pc
     aRK = aRK * (Tc / T) **0.5
     bRK = 0.08664 * (R * Tc / pc)
     return p * v ** 3 - R * T * v ** 2 + ( aRK - p * bRK ** 2 - R * T * bRK) * v - aRK * bRK
```

Figure 4: Using Redlich-kwong equation of state.

Here, the function specificvol(v) defines the problem which we wish to solve.
Step 2: Now, we have to test the function specificvol by issuing the print command and we getthe required result.


Equation of state using python
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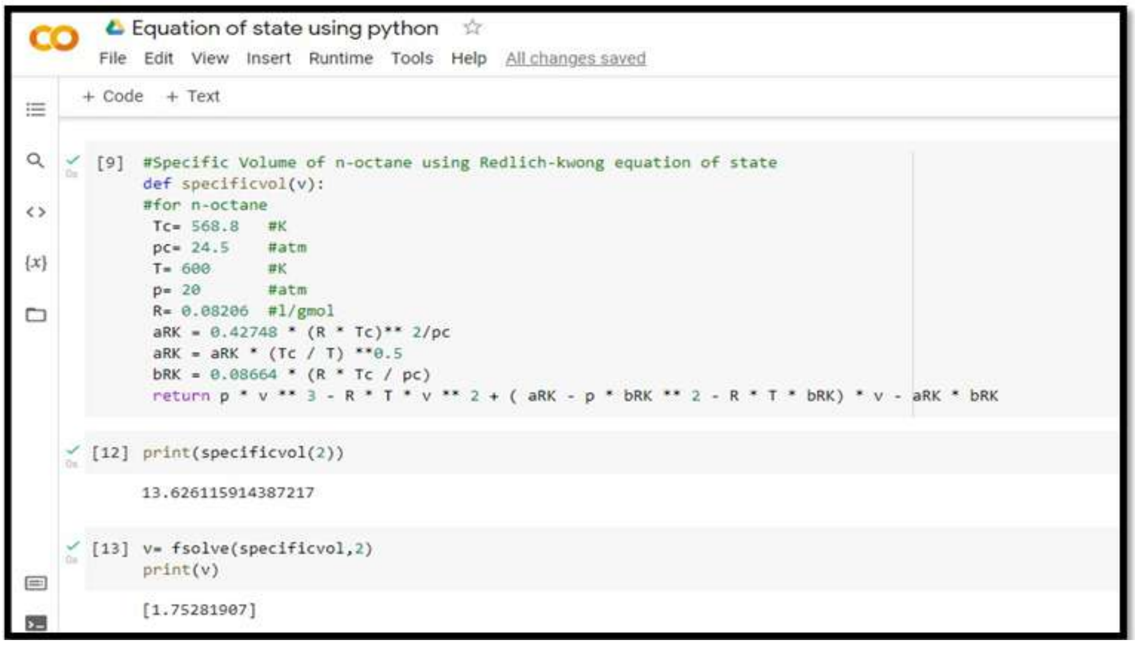
```
[9] #Specific Volume of n-octane using Redlich-kwong equation of state
    def specificvol(v):
    #for n-octane
     Tc= 568.8   #K
     pc= 24.5    #atm
     T= 600      #K
     p= 20       #atm
     R= 0.08206  #l/gmol
     aRK = 0.42748 * (R * Tc)** 2/pc
     aRK = aRK * (Tc / T) **0.5
     bRK = 0.08664 * (R * Tc / pc)
     return p * v ** 3 - R * T * v ** 2 + ( aRK - p * bRK ** 2 - R * T * bRK) * v - aRK * bRK

[12] print(specificvol(2))

     13.626115914387217
```

Figure 5: Testing the function.

The specificvol function causes python to compute the value of the function specificvol when v=2 and we get 13.626115914387217 which is correct.

Step 3: Next, we have to issue the command which solve the function specificvol.


Equation of state using python
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```
[9]  #Specific Volume of n-octane using Redlich-kwong equation of state
     def specificvol(v):
     #for n-octane
      Tc= 568.8    #K
      pc= 24.5     #atm
      T= 600       #K
      p= 20        #atm
      R= 0.08206   #l/gmol
      aRK = 0.42748 * (R * Tc)** 2/pc
      aRK = aRK * (Tc / T) **0.5
      bRK = 0.08664 * (R * Tc / pc)
      return p * v ** 3 - R * T * v ** 2 + ( aRK - p * bRK ** 2 - R * T * bRK) * v - aRK * bRK
```

```
[12] print(specificvol(2))

     13.626115914387217
```

```
[13] v= fsolve(specificvol,2)
     print(v)

     [1.75281907]
```

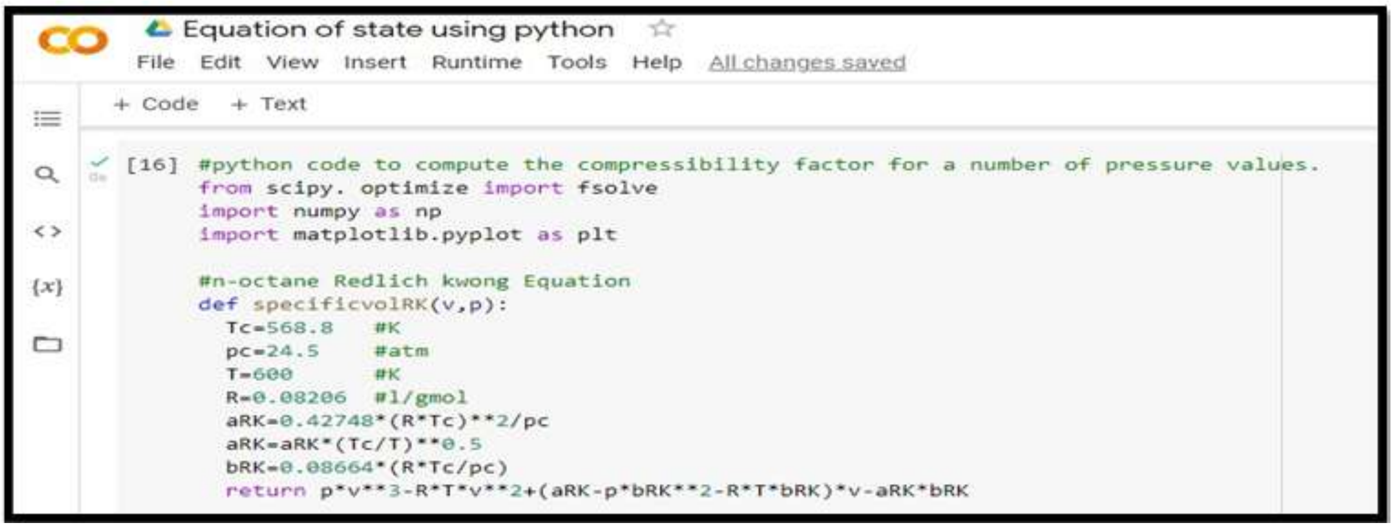
Figure 6: Issue the command to solve the function.

Hence, we get the required result 1.75281907. In specificvol function the 2 is the initial guess ofthe answer.

Example 2: Rearrange the python code to compute the compressibility factor for a number of pressure values. The following equation defined the compressibility factor:

$$Z = \frac{pv}{RT}$$

When the gas is ideal, the pressure is low and the compressibility factor will be close to 1.00. Compressibility factor will increase with increase in pressure. The following below code solves for the Redlich-kwong, Redlich-Kwong-Soave, and Peng-Robinson equations of state and thus plots the compressibility factor versus pressure. [4]


Equation of state using python
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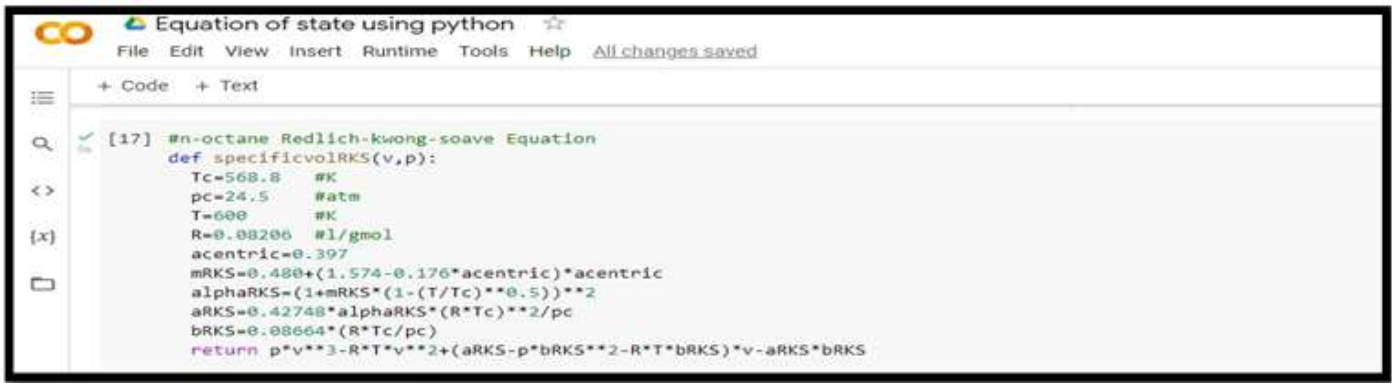
```
[16] #python code to compute the compressibility factor for a number of pressure values.
     from scipy. optimize import fsolve
     import numpy as np
     import matplotlib.pyplot as plt

     #n-octane Redlich kwong Equation
     def specificvolRK(v,p):
       Tc=568.8    #K
       pc=24.5     #atm
       T=600       #K
       R=0.08206   #l/gmol
       aRK=0.42748*(R*Tc)**2/pc
       aRK=aRK*(Tc/T)**0.5
       bRK=0.08664*(R*Tc/pc)
       return p*v**3-R*T*v**2+(aRK-p*bRK**2-R*T*bRK)*v-aRK*bRK
```

Figure 7: Compute the compressibility factor.

The above python code is for Redlich-kwong equation of state.


Equation of state using python
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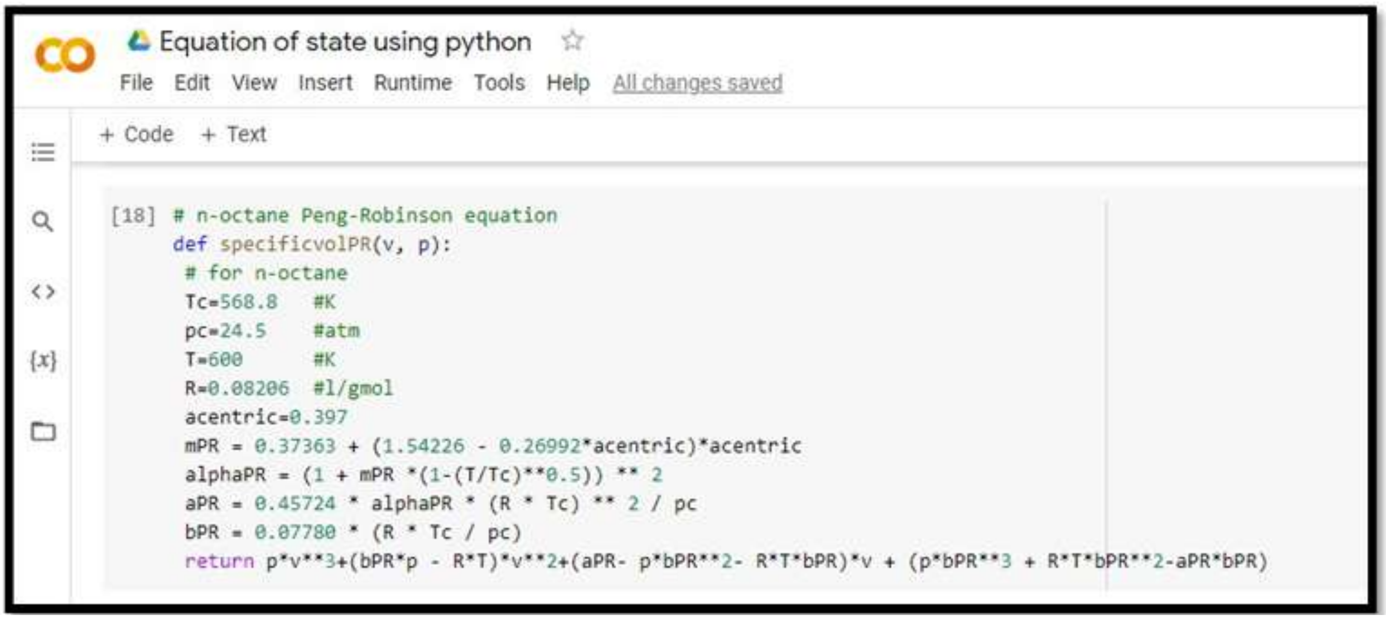
```
[17] #n-octane Redlich-kwong-soave Equation
     def specificvolRKS(v,p):
       Tc=568.8    #K
       pc=24.5     #atm
       T=600       #K
       R=0.08206   #l/gmol
       acentric=0.397
       mRKS=0.480+(1.574-0.176*acentric)*acentric
       alphaRKS=(1+mRKS*(1-(T/Tc)**0.5))**2
       aRKS=0.42748*alphaRKS*(R*Tc)**2/pc
       bRKS=0.08664*(R*Tc/pc)
       return p*v**3-R*T*v**2+(aRKS-p*bRKS**2-R*T*bRKS)*v-aRKS*bRKS
```

Figure 8: Python code for Redlich-Kwong -Soave equation of state.

The above python code is for Redlich-kwong-soave equation of state.


Equation of state using python
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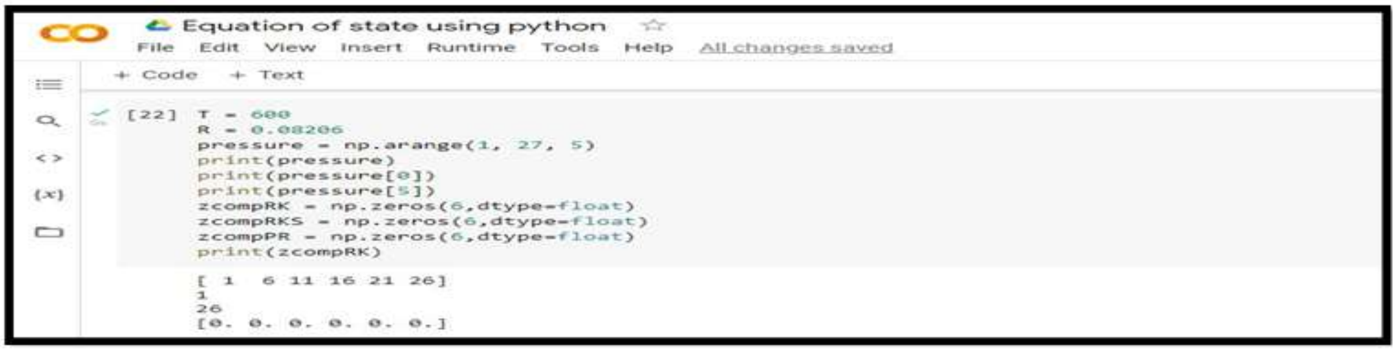
```
[18] # n-octane Peng-Robinson equation
     def specificvolPR(v, p):
      # for n-octane
      Tc=568.8    #K
      pc=24.5     #atm
      T=600       #K
      R=0.08206   #l/gmol
      acentric=0.397
      mPR = 0.37363 + (1.54226 - 0.26992*acentric)*acentric
      alphaPR = (1 + mPR *(1-(T/Tc)**0.5)) ** 2
      aPR = 0.45724 * alphaPR * (R * Tc) ** 2 / pc
      bPR = 0.07780 * (R * Tc / pc)
      return p*v**3+(bPR*p - R*T)*v**2+(aPR- p*bPR**2- R*T*bPR)*v + (p*bPR**3 + R*T*bPR**2-aPR*bPR)
```

Figure 9: Python code for Peng-Robinson equation of state.

The above python code is for Peng-Robinson equation of state.


Equation of state using python
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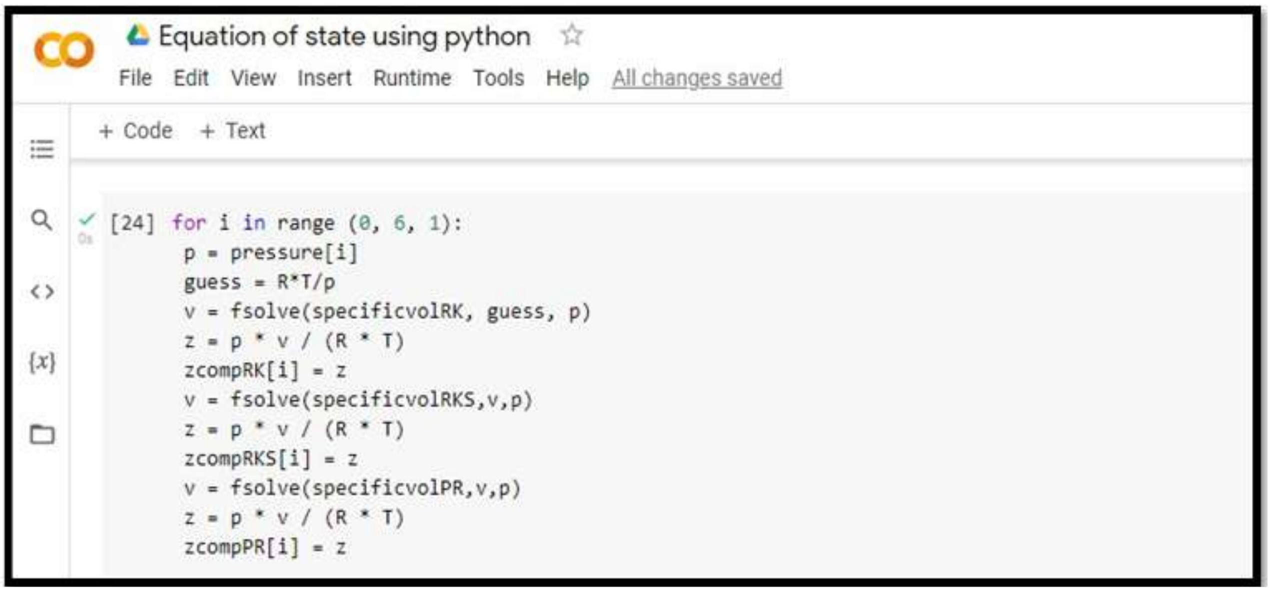
```
[22] T = 600
     R = 0.08206
     pressure = np.arange(1, 27, 5)
     print(pressure)
     print(pressure[0])
     print(pressure[5])
     zcompRK = np.zeros(6,dtype=float)
     zcompRKS = np.zeros(6,dtype=float)
     zcompPR = np.zeros(6,dtype=float)
     print(zcompRK)

     [ 1  6 11 16 21 26]
     1
     26
     [0. 0. 0. 0. 0. 0.]
```

Figure 10: Python code for Compressibility Factor equation of state.

The above python code is for Compressibility Factor equation of state.


Equation of state using python
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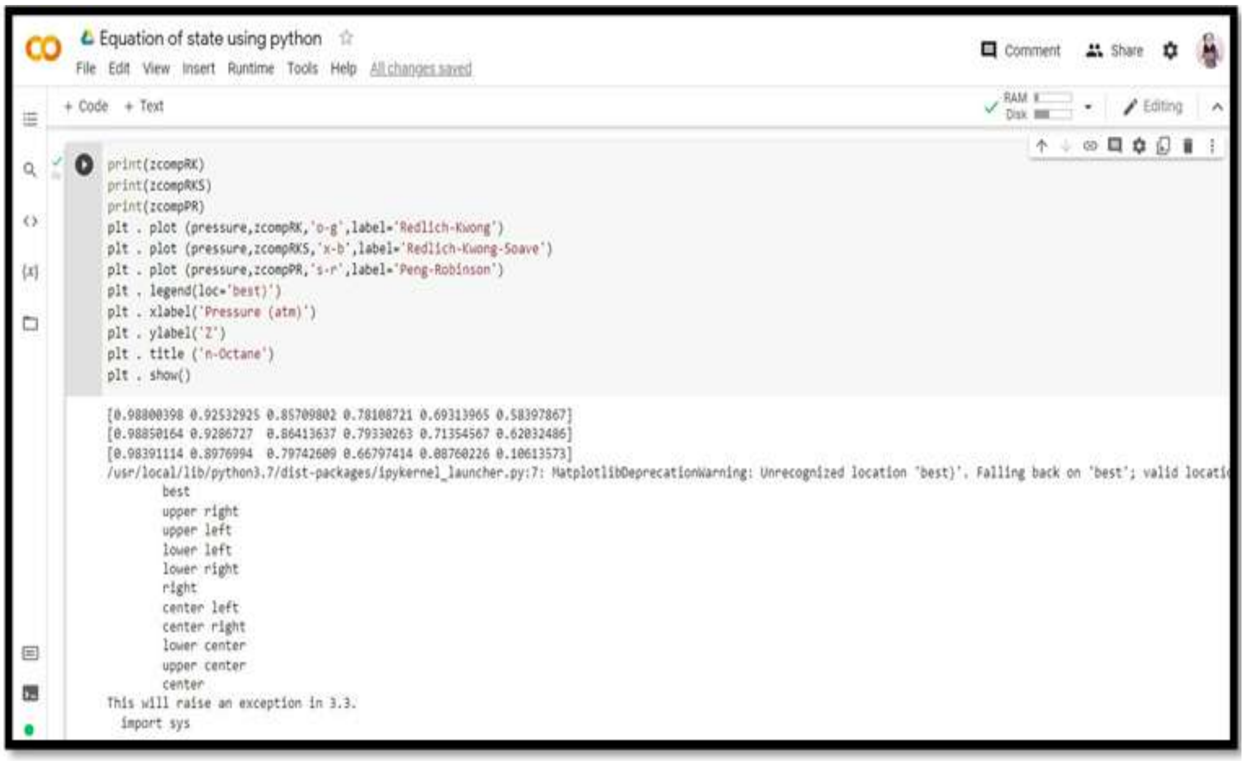
```
[24] for i in range (0, 6, 1):
       p = pressure[i]
       guess = R*T/p
       v = fsolve(specificvolRK, guess, p)
       z = p * v / (R * T)
       zcompRK[i] = z
       v = fsolve(specificvolRKS,v,p)
       z = p * v / (R * T)
       zcompRKS[i] = z
       v = fsolve(specificvolPR,v,p)
       z = p * v / (R * T)
       zcompPR[i] = z
```

Figure 11: Python code for Compressibility Factor equation of state.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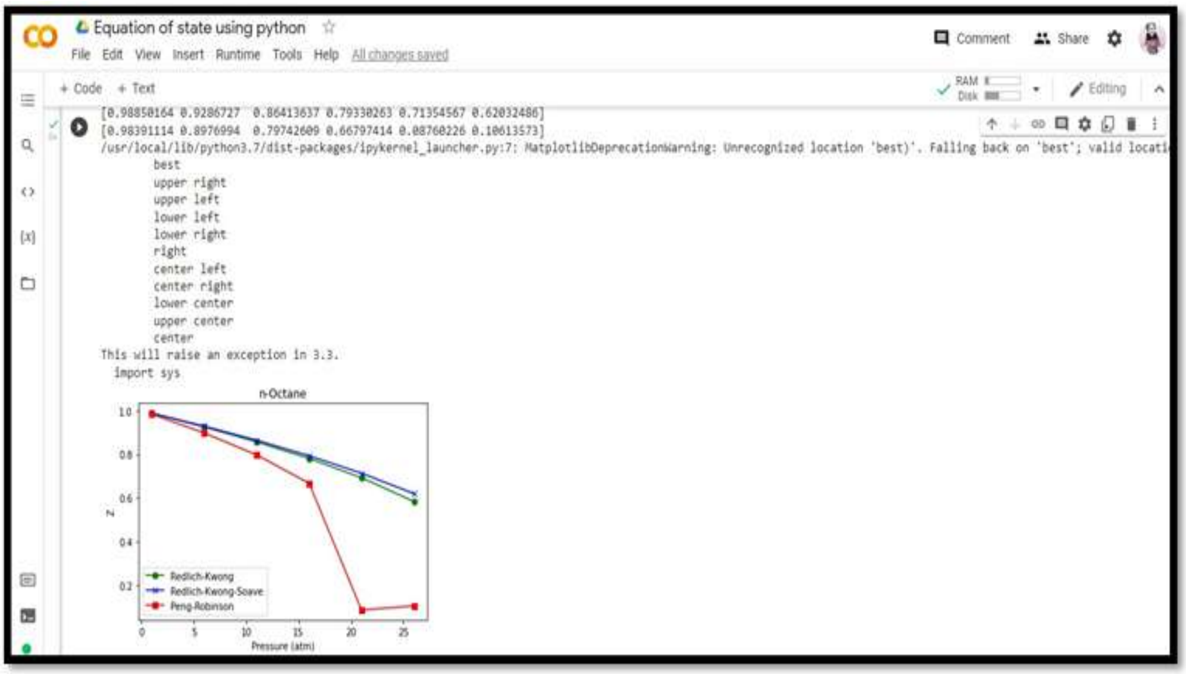
```
print(zcompRK)
print(zcompRKS)
print(zcompPR)
plt . plot (pressure,zcompRK,'o-g',label='Redlich-Kwong')
plt . plot (pressure,zcompRKS,'x-b',label='Redlich-Kwong-Soave')
plt . plot (pressure,zcompPR,'s-r',label='Peng-Robinson')
plt . legend(loc='best)')
plt . xlabel('Pressure (atm)')
plt . ylabel('Z')
plt . title ('n-Octane')
plt . show()
```

```
[0.98800398 0.92532925 0.85709802 0.78108721 0.69313965 0.58397867]
[0.98850164 0.9286727  0.86413637 0.79330263 0.71354567 0.62032486]
[0.98391114 0.8976994  0.79742609 0.66797414 0.08760226 0.10613573]
/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:7: MatplotlibDeprecationWarning: Unrecognized location 'best)'. Falling back on 'best'; valid locati
        best
        upper right
        upper left
        lower left
        lower right
        right
        center left
        center right
        lower center
        upper center
        center
This will raise an exception in 3.3.
  import sys
```

Figure 12: Python code for Compressibility Factor equation of state.


Equation of state using python
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```
[0.98850164 0.9286727  0.86413637 0.79330263 0.71354567 0.62032486]
[0.98391114 0.8976994  0.79742609 0.66797414 0.08760226 0.10613573]
/usr/local/lib/python3.7/dist-packages/ipykernel_launcher.py:7: MatplotlibDeprecationWarning: Unrecognized location 'best)'. Falling back on 'best'; valid locati
        best
        upper right
        upper left
        lower left
        lower right
        right
        center left
        center right
        lower center
        upper center
        center
This will raise an exception in 3.3.
  import sys
```

Figure 13: Python code for Compressibility Factor equation of state.

The first three commands bring in the needed routines – fsolve, numpy, and pylab (for plotting thegraph). Then there are three definitions of functions that define the equations which is governing the specific volume, Eq. (1.5) and (1.6). The main program sets the temperature, provides a vectorof 6 pressures, equidistant from 1 to 27; pressure = [1, 6, 11, 16, 21, 26]. The index goes from 0 to
5. The vectors of compressibility's are also set with 6 values for every equation of state, starting with 0. Then a loop calculation is made for "i" from 0 to 5.[5]
For each pressure in turn, the guess for the Redlich-Kwong equation of state is the result from the ideal gas law. The result from the Redlich-Kwong equation of state is used for the guess when solving the Redlich-Kwong-Soave equation of state, and that solution is used as the gues for the Peng-Robinson equation of state. For each "i", after the compressibility is found it is put in a vectorfor that equation of state. Finally, the results are plotted, with three curves on one plot.[6]

III. CONCLUSION

This paper summarize intends to solve equations of state using the Google Colab platform using Python computational language. The google Colab platform was chosen because it is free of cost, does not require the installation, setup, and configuration of Python packages and their libraries in the students' personal computers. Google Colab is a multiuser and collaborative environment, ideal for remote classes. The notebooks in the google Colab can be shared between instructor and students or between the students, which easy the communication and track of student's progress.
This paper illustrates how to solve the complicated problems and equations of states easily by writing small codes using python programming language.

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