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In [3]: # %load http://che.byu.edu/imports.py
import numpy          as np
import matplotlib.pyplot as plt
%matplotlib inline
from scipy.optimize    import fsolve, curve_fit
from scipy.integrate   import odeint, quad
from scipy.interpolate import interp1d
from scipy.misc        import derivative
import scipy.constants as const
import sympy           as sp
sp.init_printing()
import glob
import time
#import pint; u = pint.UnitRegistry()
```

This is an example of CO2 using the SRK Equation of State

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In [5]: Tc = 304.2          # Critical Temperature in K
Pc = 72.9                  # Critical Pressure in atm
R = 0.08206                # Universal Gas Constant in liter-atm/mol-K
a = 0.42747*(R*Tc)**2/Pc   # The "a" parameter in the SRK equation
b = 0.08664*(R*Tc)/Pc     # The "b" parameter in the SRK equation
omega = 0.225              # Pitzer acentric factor from Table
m = 0.48508 + 1.55171*omega - 0.1561*omega**2 # The "m" parameter in the SRK equation

T = 400                    # The system temperature in K
P = 50                     # The system pressure in atm

Tr = T/Tc                  # The reduced temperature
alpha = (1 + m*(1-Tr**0.5))**2 # The alpha in the SRK equation

print (a,b,m,Tr,alpha)    # Print the values of a,b,m,Tr,alpha

Videal = R*T/P             # Calculate the volume in liters from ideal gas law

print(Videal)              # Print the volume from the ideal gas law

def g(x) :                 # This is the function evaluation,
    return P - R*T/(x - b) + a*alpha/(x*(x+b)) # Fsolve finds the zero of the function
V = fsolve(g,Videal)       # Fsolve finds the zero of the function

print(V,g(V))              # Print the value of V in liters

3.6539244003896534 0.0296675469037037 0.8263121875 1.314924391847469 0.7722520745415591
0.65648
[0.60109199] [5.82645043e-13]
```

tm/(K-gmole)
tion
tion
5.3-1
tion

a
om the ideal gas equation
as equation

LHS - RHS of SRK equation
tion $g(V)$ with current T & P