Department of Chemical Engineering
University of California, Santa Barbara

Chemical Engineering 180A
Analysis of CO_2 and He Compressibilty at High Pressures

Wesley Johanson, Chase Hartsell, Qiye Hu
University Of California, Santa Barbara
Group 3W
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Abstract

Gaseous compressibility is a key consideration for accurate engineering calculations in many applications. In this report, the compressibility factors of CO_2 and helium were investigated using Burnett's isothermal pressure ratio method at 10°, 20°, and 30° C. The compressibility factor Z_{CO_2} was found to have a decreasing linear trend with increasing pressure, with the lowest value Z = 0.6 +/- 0.02 at 760 psi, and the system became more ideal with Z = 1 +/- 0.08 as pressure decreased to atmospheric. Helium exhibited ideal behavior, with Z_{He} being relatively ideal with Z = 1 +/- 0.1 regardless of pressure. Although no significant deviations from ideality were observed from helium gas, there is a slight positive deviation with temperature increase, showing a temperature dependence in the second virial coefficient B(T) in helium gas, in addition to CO_2. The second virial coefficients, which deviated by 50-100% from literature values, increased non-linearly with temperature, and were negative for temperatures below 20° C for helium and at all temperatures measured for CO_2. CO_2's decreasing compressibility factor with pressure highlights the implications of non-ideality in gases, and the calculations for CO_2 wouldn't be as accurate at same temperature and pressure as its ideal counterpart helium.

Introduction

With recent world events and supply chain issues, supply storage has became a major concern in the United States. Many vital instruments, like MRI machines in hospitals, require liquid helium for cooling purposes. However, with the recent turmoil in one of the world's major helium suppliers, helium has become scarce[1] and this shortage could potentially derail scientific and medical research. In lieu of this, finding new compressible gasses may prove to be important for future applications in this sense. The goal of this report is to find the compressibility factor Z for gases CO_2 and Helium, and to create a solid model for z at different temperatures. The pressure, molar volume, and temperature of a gas are related by the equation of state:

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

where R is the universal gas constant. The compressibility factor, Z, is a unit-less measure of gas ideality (ideal gas has Z =1), and it can be determined for different gasses at different conditions. Factors that affect gas ideality include inter-molecular forces and molecular size. Because of this, ideal behavior is observed at high temperatures and low pressures, when these two effects are minimized. To measure the compressibility factors of carbon dioxide and helium, we employed Burnett's method[2] and observed the change in pressure as a gas was expanded at a constant temperature. By relating the change in pressure after the r^{th} expansion to a consistent change in volume (represented by the apparatus constant, N), the deviations from ideal expectations can be measured.

$$\frac{p_{r-1}}{p_r} = N\frac{Z_{r-1}}{Z_r} \tag{2}$$

Because gas acts closest to ideal at low pressures, taking the limit as pressure goes to zero allows us to solve for the apparatus constant. Using this, a relation can be developed between the ratio in pressures after an expansion to the ratio in compressibility factors. We can then calculate Z from the initial and current pressure at any given expansion.

$$p_r N^r = \left(\frac{p_0}{Z_0}\right) Z_r \tag{3}$$

Because compressibility is also affected by temperature, a linear model can be generated to obtain Z as a function of pressure at each isotherm. The slope of this line is the temperature dependent B'; the intercept, at zero pressure, is Z=1: an ideal gas.

$$Z = 1 + B'P \tag{4}$$

From the slope of compressibility factor B', the second virial coefficient can be obtained from B' through equation[3]:

$$B(T) = B' * RT \tag{5}$$

However, due to unique molecular structures, the compressibility and second virial coefficient would deviate from ideal state as pressure increases. This is due to multiple factors from intermolecular forces. The attractive and repulsive behavior between the pure gas molcules, like the Van der Waals forces, would affect how ideally a molecule like methane would behave under a set temperature and pressure[4].

Experimental Methods

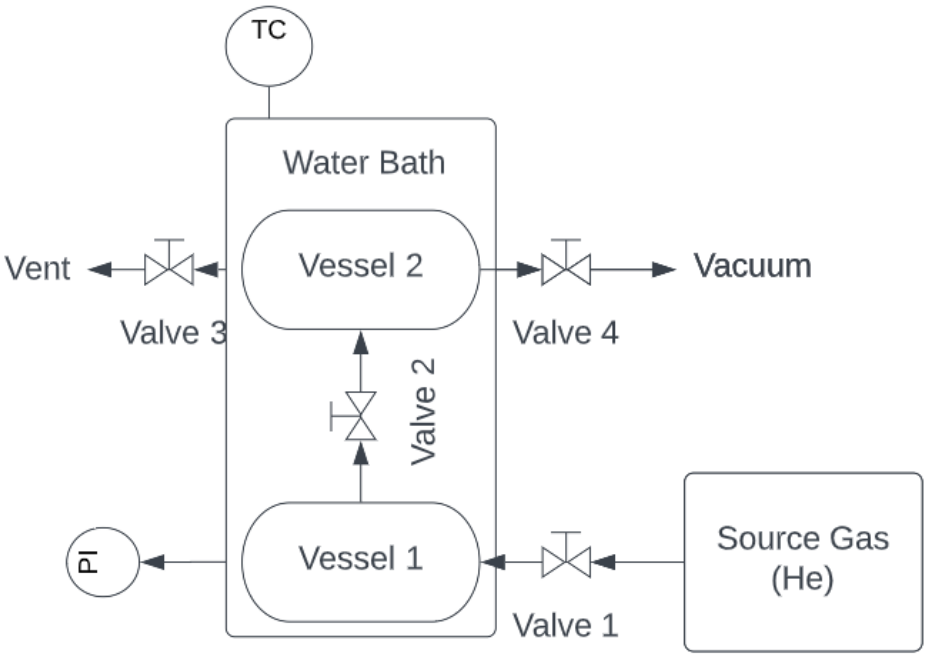

Figure 1: Pressure vessel apparatus where gas was expanded and the pressure was recorded after it reached equilibrium.

The apparatus (Figure 1)consists of a high purity gas source (He and CO_2, Airgas, 100%). The high purity gas source is connected to two interconnected vessels, one of which is attached with a pressure indicator (PI) and the other to vent and vacuum. All the connections connected to the vessels are regulated with a manual gate valve, with the whole apparatus taking place in a temperature controlled (TC) water bath.

The goal of this experiment is to use Burnett's method to find the compressibility factor Z of gases He and CO_2, at different pressure and temperature. A source gas, CO_2 or He, is introduced into the vacuumed vessel 1 via opening valve 1.

Once the set pressure is reached in vessel 1, valve 1 is closed and valve 2 is opened slowly to allow gas to expand into the vacuumed vessel 2 isothermally. Once the pressure equalized, it is recorded and valve 2 is closed and the gas in vessel two is vented out via valve 3 and vacuumed via valve 4. After vessel 2 is vacuumed, valve 2 is reopened for another expansion. Expansions are repeated until the equilibrium pressure approaches atmospheric pressure, or the measurement is too low to accurately read. With the expansion data at different temperature, the compressibility factor can be calculated via equation 2 and 3, thus a pressure dependent compressibility value Z graph is made (Figures 2 & 3). The slope of the Z graph is the temperature dependent second virial coefficient, which is graphed at the three temperatures measured (Figure 4).

Results and Discussion

The Z factors as a function of pressure for helium and carbon dioxide (Figures 2 & 3), exhibit a linear dependence in this pressure range. Values for raw pressure readings used to calculate Z are located in Tables 1 & 2 in Appendix A. The compressibility factor for helium does not have a clear trend with increasing pressure. There is imprecise correlation between pressure and the Z factor given by the low R^2 values at three different temperatures, however the error bars suggest relative ideality with Z = 1 +/- 0.1 (Figure 2). Gas is most ideal at high temperatures and low pressures, however the 30° isotherm exhibits the most deviation from ideal behavior, even outside of the error range for most measurements. ADD MORE

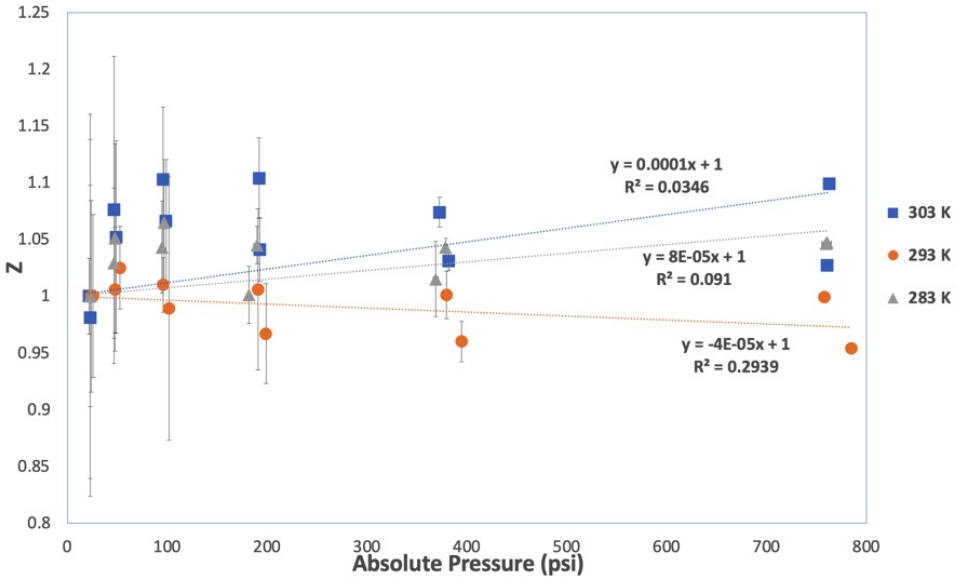

Figure 2: Compressibility of helium at 3 isotherms. Error bars represent standard error of calculations and pressure gauge readings.

The seemingly unpredictable points shown in Figure 2 can be explained by Helium's inert nature. Due to helium's monoatomic and stable nature from filled orbitals, helium atoms have no attraction towards each other, making it inert. Helium is also the second smallest atom, so the volume of the container is a very fair estimate for the volume of empty space, whereas the larger carbon dioxide makes a more significant effect on this assumption. This explains the ideal behavior seen in Figure 2. Even with the imprecise distribution, Z_{He} has a value of relatively one across all pressures. This is similar to Imbert's Z value of 1 + 0.0045 P(MPa)[5]. The cause of the high spread in these values, especially at lower pressures, is because error in the pressure readings gets propagated through after each expansion. In addition to this, the gauge was accurate to +/- .25%, and this systematic error also becomes more significant at lower pressure readings. Because helium was so close to ideal, these deviations look like a large spread with little correlation however the error bars suggest a linear pressure dependence at these conditions.

In addition to helium, a trend for Z_{CO_2}'s compressibility is also reasonable. However, the Z factors for carbon dioxide show a stronger pressure dependence, decreasing linearly in this temperature and pressure range (Figure 3). CO_2's bonds provided the molecule with a net zero dipole, but compared to helium's inert nature, CO_2 experiences bigger Van der Waals forces due to the instantaneous dipole moment given by a more electronegative oxygen atom at each end. This means that when a molar charge is introduced into a constant volume, CO_2 gas molecules experience a stronger attractive force, exhibiting a lower pressure than ideal and thus having a lower Z value at these pressures. The trends shown in Figure 3 also match with Sage and Lacy (1955) and Burton Technical Bulletin (1990) data showing a negative linear slope in the Z factor until 1500 psia at 100°F[6]. Experimental data also shows the same negative slope, with the similar Z values within 4%. Experimental data also displays ideal gas trends, with the higher temperature exhibiting the most ideal behavior.

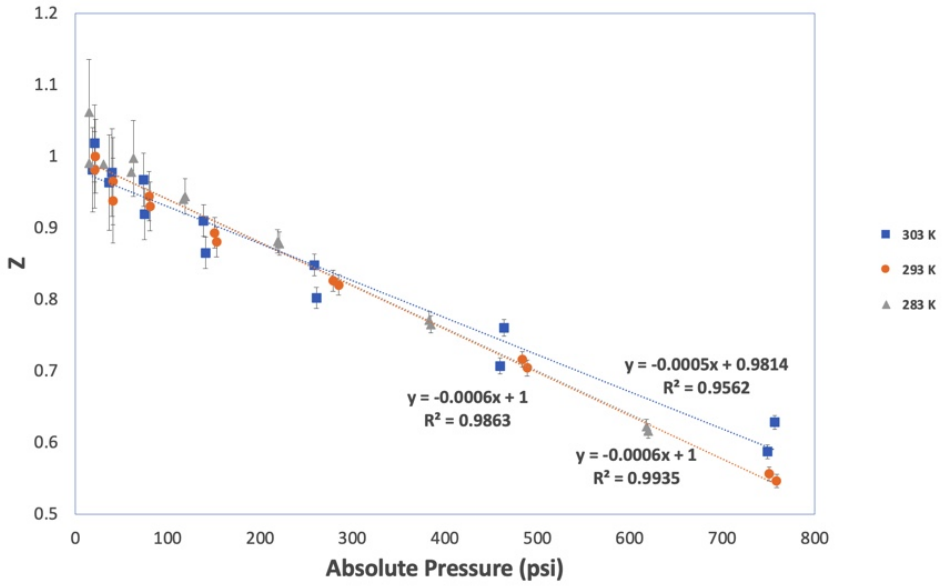

Figure 3: Compressibility of carbon dioxide at 3 isotherms. Error bars represent standard error of calculations and pressure gauge readings.

A key difference in the Z factor determination between helium and carbon dioxide gas is that carbon dioxide would readily liquefy under high pressure. From the CO_2 phase diagram, CO_2 liquefies at 30°C and 760 psi, and at 10°C it liquefies at 650 psi. This prevented us from charging the vessel with as much gas, and one less expansion was able to be precisely measured at 10°C. ADD MORE

After obtaining experimental data for the compressibilty factors of each gas, a linear regression model was set up, with the intercept set at the ideal Z = 1. Using this isothermal variation of the pressure ratio method to determine Z factors, the slope of these lines (Figure 4) are the second virial coefficients, which are dependent on temperature[7]. ADD MORE, explain values and comparison/physical stuff that affects B

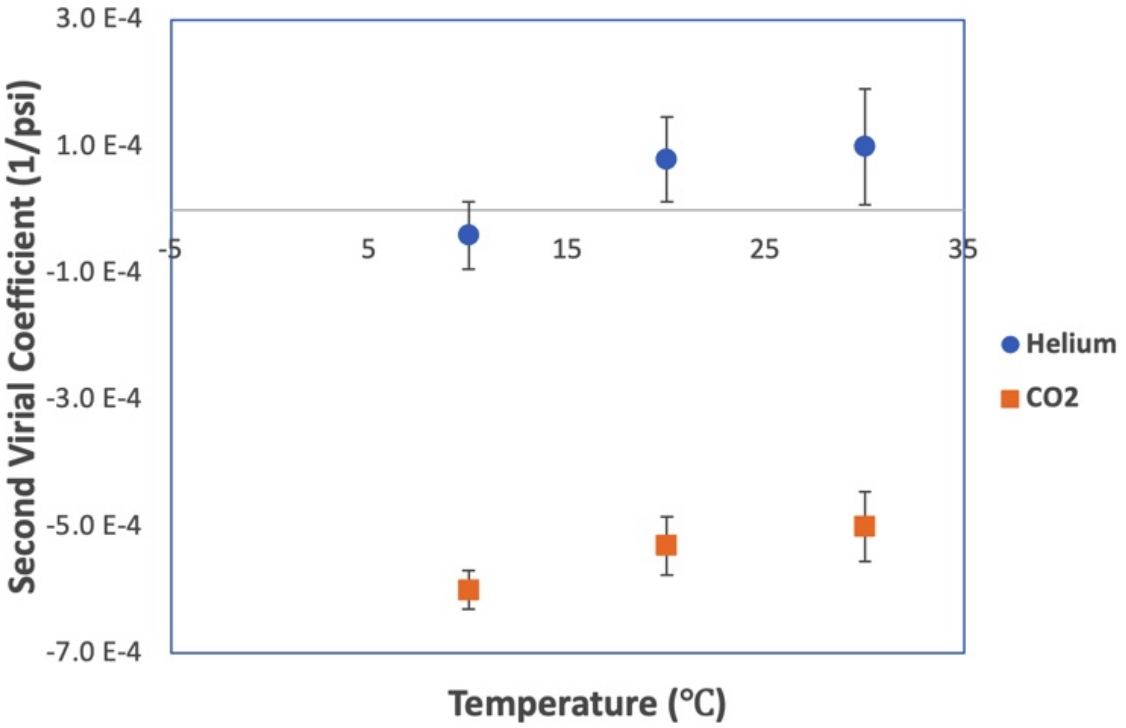

Figure 4: The second virial coefficients of helium and carbon dioxide at the three temperatures that were measured. Error bars represent standard error of the values calculated over two trials of six expansions at each isotherm.

Conclusion

The chemical make-up of a gas affects how compressible it is under high pressure. CO_2's compressibility decreased with increasing pressure at all three isotherms. The compressibility factor Z_{CO_2} has decreased down to almost 0.6 at 750 psi, meaning that at same pressure and volume, CO_2 contains 40% more moles than helium according to equation 1. The decrease in Z_{CO_2} is a result of the Van der Waals attraction between the molecules, and as molecules being compressed, they would have less expulsion forces between each other as experienced on helium gas. In addition, CO_2 is a significantly larger molecule than monoatomic helium, and the fact that a vessel of CO_2 has less empty space between the gas particles than helium has implications on its compressibility.

References

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Appendix A: Raw Data

Figure 4 displays how N, the apparatus constant, was experimentally determined. N is the ratio of final volume to initial volume for each expansion, and it was constant for each expansion. Vessel 1 and 2 theoretically had the same volume, so the apparatus constant was expected to be two, and the average of both gas's calibration proved this to be believable within the error range.

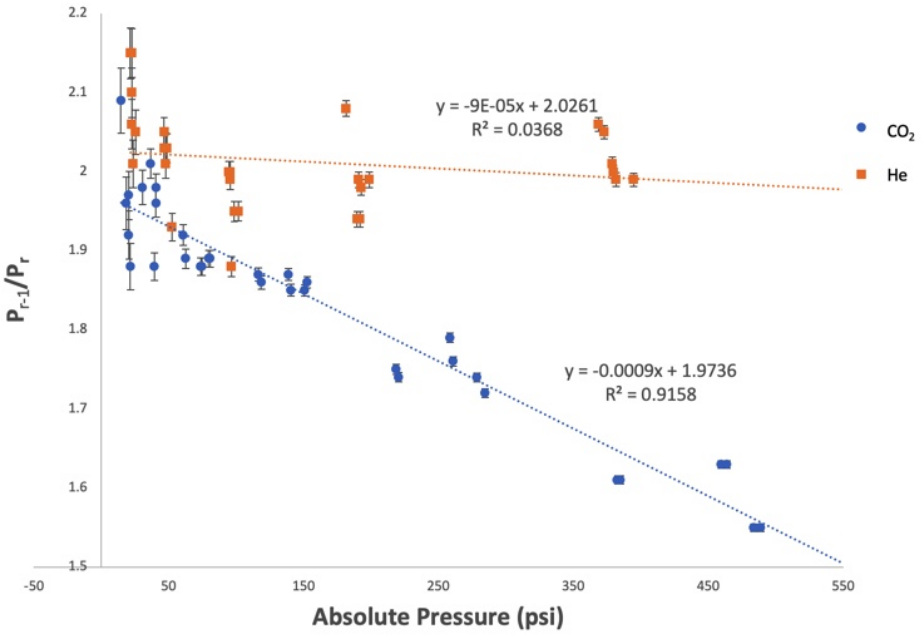

Figure 5: Calibration for the apparatus constant of the helium pressure vessel system. The limit as pressure approaches 0 (which is the y-intercept) determines the apparatus constant N i.e. the ratio of V_r/V_{r-1}. This was determined on the same apparatus with helium and carbon dioxide, and the expected value is 2.

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To determine Z_0 for each run, regression was used to find the limit of our data as gauge pressure approached zero. This gives the ratio of the $\frac{P_0}{Z_0}$, so that successive Z factors can be calculated using equation 6 (Appendix B).

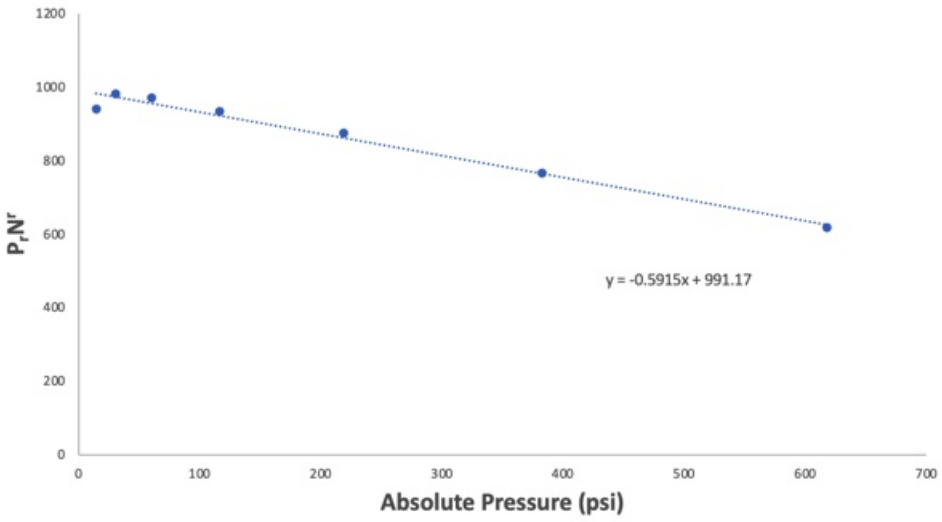


Figure 6: As P_r approaches low pressures, the value of Z_r approaches unity. The limit of this data set as pressure approaches atmospheric allows us to determine the value of Z_0 in equation 3. The data in this graph is from the 12th run (carbon dioxide at 283 K).

Table 1: Raw pressure measurements for each successive expansion at a given temperature for He. Two series of five expansions were tested for each temperature.

Species	Run [experiment #]	Expansion # (r)	Temperature [℃]	P_r[psi, guage]
He	1	0	30.4	746
He	1	1	30.2	367
He	1	2	29.9	178
He	1	3	29.9	84
He	1	4	30.1	34
He	1	5	30.1	8
He	2	0	30.1	748
He	2	1	30.1	358
He	2	2	30.1	177
He	2	3	30.1	81
He	2	4	30.1	32
He	2	5	30.1	7
He	3	0	20.1	770
He	3	1	20.1	380
He	3	2	20.1	184
He	3	3	20.1	87
He	3	4	20.1	38
He	3	5	20.1	11
He	4	0	20.1	743
He	4	1	20.1	365
He	4	2	20.1	176
He	4	3	20.1	81
He	4	4	20.1	33
He	4	5	20.1	9
He	5	0	10.2	746
He	5	1	10.3	354
He	5	2	10.4	175
He	5	3	10.4	80
He	5	4	10.5	32
He	5	5	10.6	8
He	6	0	10.2	745
He	6	1	10.2	364
He	6	2	10.3	167
He	6	3	10.2	82
He	6	4	10.3	33
He	6	5	10.3	8

Table 2: Raw pressure measurements for each successive expansion at a given temperature for $C0_2$. Two series of six expansions were tested for each temperature.

Species	Run [experiment #]	Expansion # (r)	Temperature [°C]	P_r[psi, guage]
C02	7	0	30.1	742
C02	7	1	29.9	449
C02	7	2	29.9	244
C02	7	3	30.0	124
C02	7	4	30.0	59
C02	7	5	30.0	22
C02	7	6	30.0	4
C02	8	0	30.0	734
C02	8	1	30.0	445
C02	8	2	30.0	246
C02	8	3	30.0	126
C02	8	4	30.0	60
C02	8	5	30.0	25
C02	8	6	30.0	6
C02	9	0	20.0	744
C02	9	1	20.0	474
C02	9	2	20.0	270
C02	9	3	20.0	138
C02	9	4	20.0	66
C02	9	5	20.0	26
C02	9	6	20.0	7
C02	10	0	20.0	736
C02	10	1	20.0	469
C02	10	2	20.0	264
C02	10	3	20.0	136
C02	10	4	20.0	65
C02	10	5	20.0	26
C02	10	6	20.0	6
C02	11	0	10.0	605
C02	11	1	10.0	370
C02	11	2	10.0	206
C02	11	3	10.0	104
C02	11	4	10.0	48
C02	11	5	10.0	8
C02	11	6	10.0	Unreadable
C02	12	0	10.0	603
C02	12	1	10.0	368
C02	12	2	10.0	204
C02	12	3	10.0	102
C02	12	4	10.0	46
C02	12	5	10.0	16
C02	12	6	10.0	Unreadable

Table 3: Comparison of our second virial coefficient calculations with literature values

		Virial Coefficient: Lit values			
Species	Temp	Lit (cm3/mol)	us (regression line)	us cm3 / mol	%error
C02	30	111.3	-0.0005	-182.8	64.23%
C02	20	125.6	-0.00053	-187.4	49.17%
C02	10	136.7	-0.0006	-204.9	49.87%
He	30	3.8	0.0001	36.6	862.03%
He	20	-2.2	0.00008	28.3	1185.50%
He	10	-21.7	-0.00004	-13.7	-37.06%

Appendix B: Sample Calculations

For each subsequent expansion,

$$\left(\frac{p_{r-1}}{p_r}\right) = N\left(\frac{Z_{r-1}}{Z_r}\right) \tag{6}$$

this equation was used to determine the apparatus coefficient. As low pressures are approached, the gas behaves more ideally. Consequentially the ratio of $\frac{Z_{r-1}}{Z_r}$ approaches 1 and N will be the ratio of $\frac{p_{r-1}}{p_r}$ as seen in the limit.

$$\lim_{p\to 0}\left(\frac{p_{r-1}}{p_r}\right) = N \tag{7}$$

$$p_r N^r = \left(\frac{p_0}{Z_0}\right) Z_r \tag{8}$$

This equation was used to find the value of Z_0. At low pressures, the value of Z_r approaches unity since it behaves ideally. The value of Z_0 can be determined from the the ratio of the initial pressure and $P_r N^r$.

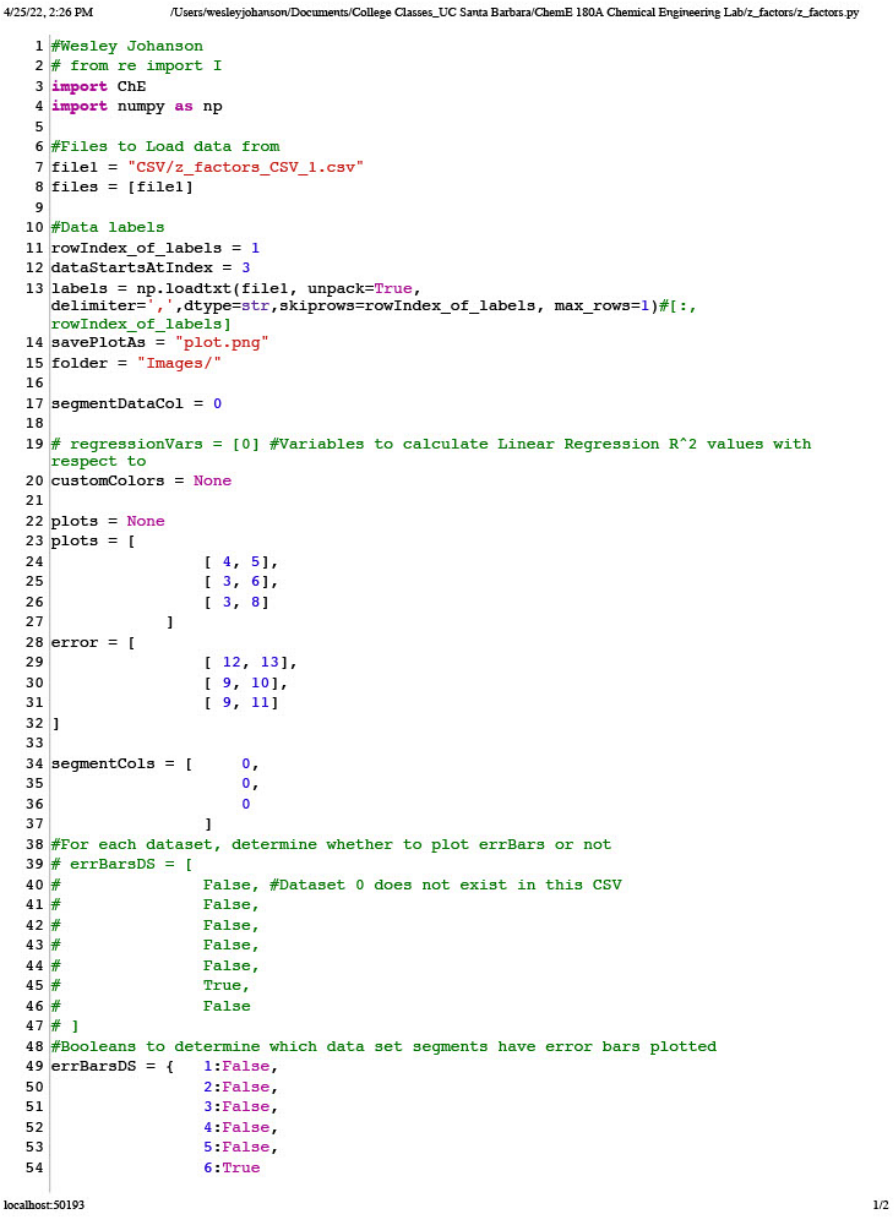
Every value recorded for pressure was within .25% of its true value according to the gauge, as well as a .5 psi uncertainty between the tick marks, and an estimate was made to best determine the observed pressure after each expansion. With this error, it gets bigger as we take the ratio of the pressure at each given expansion (calculated by the 'Multiplication or division' method).This error is carried through to calculating Z and B with the same method.

Type of calculation	Example†	Standard deviation of y
Addition or subtraction	Y=a+b-c	$S_y=(S_a^2+S_b^2+S_c^2)^{1/2}$
Multiplication or division	Y=a*b/c	$S_y/y=\{(S_a/a)^2+(S_b/b)^2+(S_c/c)^2\}^{1/2}$
Exponentiation	$Y=a^x$	$S_y/y=x\ (S_a/a)$
Logarithm	$Y=\log_{10}a$	$S_y=0.434\ (S_a/a)$
Antilogarithm	$Y=\text{antilog}_{10}a$	$S_y/y=2.303\ Sa$

† a, b, and c are experimental variables whose standard deviations are S_a, S_b, and S_c, respectively.

Figure 7: Error propagation was calculated using the methods on this chart. When combining two values with error, the propagation was kept through and error grew as we calculated Z factors for more and more expansions.

Appendix C: Program Files



4/25/22, 2:26 PM /Users/wesleyjohanson/Documents/College Classes_UC Santa Barbara/ChemE 180A Chemical Engineering Lab/z_factors/z_factors.py

```python
#Wesley Johanson
# from re import I
import ChE
import numpy as np

#Files to Load data from
file1 = "CSV/z_factors_CSV_1.csv"
files = [file1]

#Data labels
rowIndex_of_labels = 1
dataStartsAtIndex = 3
labels = np.loadtxt(file1, unpack=True,
delimiter=',',dtype=str,skiprows=rowIndex_of_labels, max_rows=1)#[:,
rowIndex_of_labels]
savePlotAs = "plot.png"
folder = "Images/"

segmentDataCol = 0

# regressionVars = [0] #Variables to calculate Linear Regression R^2 values with
respect to
customColors = None

plots = None
plots = [
                [ 4, 5],
                [ 3, 6],
                [ 3, 8]
            ]
error = [
                [ 12, 13],
                [ 9, 10],
                [ 9, 11]
]

segmentCols = [     0,
                    0,
                    0
                ]
#For each dataset, determine whether to plot errBars or not
# errBarsDS = [
#               False, #Dataset 0 does not exist in this CSV
#               False,
#               False,
#               False,
#               False,
#               True,
#               False
# ]
#Booleans to determine which data set segments have error bars plotted
errBarsDS = {   1:False,
                2:False,
                3:False,
                4:False,
                5:False,
                6:True
```

localhost:50193 1/2

Figure 8: Primary logic/script: python code

```
            }

# error = None #OVVERRIDE DELETE ME

yLabelOverride = None
# YLabels = [   "$Vz/Vz_{Max}$",
#           "friction factor",
#           "$V^{+}$",
#           "poop3"
#           ]

seg_mks = [".",".", "v", "+","^",'3','2', '3', '2']


_markers = [seg_mks for i in range(0,12)]
# print(_markers)

for file in files:
    i = 0
    for plotData in plots:
        #Make Plot Obj_____________________________________________________
        plot = ChE.ChEplot()
        plot.loadCSV_str(file, labels, indepVars=1, skip=dataStartsAtIndex)
        #Set Data__________________________________________________________
        #FOR MORE FILES THIS WILL NEED TO CHANGE
        plot.setDataLabel(labels)
        #Plotting__________________________________________________________
        plot.setDataColors(customColors)
        plot.setFxns2Plot(plotData)
        # plot.plotData_str(width=6,height=6, markers=_markers,
err=error[i],seg=segmentCols[i])
        plot.plotData_str(width=6,height=6, markers=_markers,
err=error[i],seg=segmentDataCol, pltErrBar=errBarsDS)
        #Statistics & Regression___________________________________________
        # plot.plotLRegLines(width=0.5)
        # plot.printAllRSquared()

        #Plot Parameters___________________________________________________
        xaxisLabel = labels[plotData[0]] #Don't Change
        yaxisLabel = yLabelOverride[i] if yLabelOverride else labels[plotData[1]]
        plot.setAxisLabels(xaxisLabel, yaxisLabel, xpadding=5, ypadding=5)
        plot.setTicProps()
        # plot.setNumTics(delta_x=10, delta_y=10, x_subTics=3, y_subTics=3)
        plot.showLegend()
        # plot.changeFont()

        #Presentation______________________________________________________
        # plot.showPlot()
        temp = folder + str(i) + '_' + savePlotAs
        plot.savePlot(filename=temp,_dpi=600)
        print(temp)
        plot.close()
        i += 1

print("Program Complete")
```


Figure 9: Primary logic/script: python code

```python
#Wesley Johanson
# from aifc import _Marker
# from re import I
from pprint import pprint
from re import I
import matplotlib as mpl
import matplotlib.pyplot as plt
import numpy as np
import matplotlib.font_manager as fm
from sklearn.linear_model import LinearRegression
from scipy import stats
import random
import sys

# sys.path.append("/Users/wesleyjohanson/Documents/Python_Modules")
class ChEplot:
    def __init__(self):
        self.figure=None
        self.dataLabels=None
        self.dataColors=None
        #Counting Elements
        self.numDataVars=None
        self.numDataFns=None
        self.numDataSets=None
        self.data=None
        self.fxns2plot=None




    def loadCSV_str(self, filename: str, names: list, indepVars, skip=0):
        """Loads each column of data from the CSV file into a row of a numpy
        array stored in self.data

        'names' is a list of names for the data sets in each col of the CSV"""
        # if indepVars < 1 or indepVars > len(names): return
        self.data = np.loadtxt(filename, unpack=True, delimiter=',',skiprows=skip,
dtype=str)
        # if indepVars > self.numDataSets: self.data = none; return
        self.dataLabels = names
        self.numDataVars = indepVars
        self.numDataSets = len(self.data)
        self.numDataFns = self.numDataSets - self.numDataVars
        # for col in range(0, len(self.data)):
        #   new_x = []
        #   new_y = []
        #   for row in range(0, len(self.data[0])):
        #       if self.data[col,row] != "":
        #           new_x.append(float(self.data[col,row]))
        #           new_y.append(float(self.data[0,row]))



    #LEGACY
    def setData(self, data: list, vars=1):
        "Replaces Data and performs same operations as loadCSV"
        self.data = data
```


Figure 10: Plotting Class python code

```
57          self.numDataVars = vars
58          self.numDataSets = len(self.data)
59          self.numDataFns = self.numDataSets - self.numDataVars
60
61
62      #Printers
63      def printAllData(self):
64          print(
65              "\n",self.figure
66              ,"\n",self.dataLabels
67              ,"\n",self.numDataVars
68              ,"\n",self.numDataFns
69              ,"\n",self.numDataSets
70              ,"\n",self.data
71              ,"\n",self.fxns2plot)
72          "print all data points in self.data"
73          print(self.data)
74
75      def printMeans(self):
76          "Prints the  mean value of each row vector in self.data"
77          for i in range(0, self.numDataSets):
78              outputStr = "the mean of "
79              if self.dataLabels[i] is not None:
80                  outputStr += self.dataLabels[i]
81              outputStr += "\t\tis " + str(np.mean(self.data[i]))
82
83      #Setters
84      def setDataLabel(self, names):
85          """
86          Stores a list of strings into the instance, where each str in the list
87          is the name of the corresponding column in the CSV file
88          """
89          self.dataLabels = names
90
91      def segmentData(self):
92          pass
93
94      def setLRegLineColors(self, colors=[]):
95          self.LRegLineColors = colors
96
97      def setIndepVars(self, vars):
98          "Vars are the first arrays in the self.data matrix"
99          self.setIndepVars = vars
100
101     #Plotters
102     @staticmethod
103     def randColor():
104         return "#"+''.join([random.choice('0123456789ABCDEF') for j in range(6)])
105
106     def plotData_str(self, width, height, markers=None, err=None, xScale="", yScale="",
    seg=None, pltErrBar=False):
107         self.figure = plt.figure(figsize=(width, height))
108         L, B, W, H = [0.15, 0.1, 0.80, 0.85]
109         self.figure.axis = []
110         self.figure.axis.append(self.figure.add_axes([L, B, W, H]))
111         var = self.fxns2plot[0]
112         for fn in self.fxns2plot[1:]:
113             #Segment the data if neccessary
```


Figure 11: Plotting Class python code

```
114                 if seg is not None:
115                     #Make a dictionary, for each dataset index, make a blank array
116                     # print(self.data[seg])
117                     segSet = [int(s) for s in self.data[seg]]
118                     segSet = set(segSet)
119                     segSet = list(segSet)
120                     # print("segSet = ", segSet)
121                     Xseg = { i:[] for i in segSet}
122                     Yseg = { i:[] for i in segSet}
123                     Xseg_err = { i:[] for i in segSet}
124                     Yseg_err = { i:[] for i in segSet}
125                     # print("Xseg = ", Xseg)
126 
127                     #add the data, remove blank string elements
128                     for i in range(0,len(self.data[var])):
129                         # print("AT LOC I = ", self.data[seg][i])
130                         if (self.data[var][i] != "" and self.data[fn][i] != ""):
131                             Xseg[int(self.data[seg][i])].append(self.data[var][i])
132                             Yseg[int(self.data[seg][i])].append(self.data[fn][i])
133                             Xseg_err[int(self.data[seg][i])].append(float(self.data[err[0]]
    [i]))
134                             Yseg_err[int(self.data[seg][i])].append(float(self.data[err[1]]
    [i]))
135 
136                     # print("Xseg\n",Xseg)
137                     # print("Yseg\n",Yseg)
138 
139                     for i in segSet:
140                         #REMOVE ME
141                         # if i !=3: continue
142                         x = Xseg[i]
143                         y = Yseg[i]
144                         lbl = self.dataLabels[fn] + "_" + str(i)
145                         new_x = [float(i) for i in x]
146                         new_y = [float(i) for i in y]
147                         x_error = Xseg_err[i]
148                         y_error = Yseg_err[i]
149                         #Add the datasets index to the label
150                         # lbl = lbl + "_" + str(i)
151                         #Set markers for plotting
152                         if markers is not None:
153                             #"modified for the segmented data"
154                             mk = markers[fn][i]
155                         else:
156                             mk = "."
157 
158                         #Colors
159                         if self.dataColors is not None:
160                             # clr = self.dataColors[fn]
161                             clr = ChEplot.randColor()
162                             self.figure.axis[0].plot(new_x,new_y,mk,label=lbl,color=clr)
163                         else: #I don't think this condition is possible anymore
164                             self.figure.axis[0].plot(new_x,new_y,mk,label=lbl)
165                         #ERROR BARS MODIFY THIS FOR SEGMENETED DATA
166                         if err is not None and pltErrBar[i] is True:
167                             #$plt.errorbar(new_x, new_y, xerr=x_error, yerr=y_error)
168                             #DELETE THIS LINE, TESTING
169                             # if i != 5: continue
```


Figure 12: Plotting Class python code

```
                        self.figure.axis[0].errorbar(new_x, new_y, xerr=x_error,
yerr=y_error ,linewidth=0.9) #,ecolor=None) # fmt='none')
                    # else:
                    #   print("ERROR BARS ARE NOT PLOTTED FOR", err, "\n", pltErrBar[i])
                    #Scale
                    if xScale=="log":
                        self.figure.axis[0].set_xscale('log')
                    if yScale=="log":
                        self.figure.axis[0].set_yscale('log')

#No segmentation
            else:
                x = self.data[var]
                y = self.data[fn]
                lbl = self.dataLabels[fn]
                #Remove Data points with blank strings that don't map to floats
                for col in range(0, len(self.data)):
                    new_x = []
                    new_y = []
                    x_error = []
                    y_error = []
                    for row in range(0, len(self.data[0])):
                        if self.data[col,row] != "" and self.data[var,row] !="":
                            if err is not None:
                                x_error.append(float(self.data[err[0], row]))
                                y_error.append(float(self.data[err[1], row]))
                            new_x.append(float(self.data[var,row]))
                            new_y.append(float(self.data[col,row]))
                #Set markers for plotting
                if markers is not None:
                    mk = markers[fn]
                else:
                    mk = "."
                #Colors
                if self.dataColors is not None:
                    clr = self.dataColors[fn]
                    self.figure.axis[0].plot(new_x,new_y,mk,label=lbl,color=clr)
                else: #I don't think this condition is possible anymore
                    self.figure.axis[0].plot(new_x,new_y,mk,label=lbl)
                #ERROR BARS
                if err is not None:
                    plt.errorbar(new_x, new_y, xerr=x_error, yerr=y_error, )
                #Scale
                if xScale=="log":
                    self.figure.axis[0].set_xscale('log')
                if yScale=="log":
                    self.figure.axis[0].set_yscale('log')

    def plotLRegLines(self, width=0.5, style='-'):
        var = [float(x) for x in self.data[0]]
# self.fxns2plot[0]
        # fxns = self.fxns2plot[1:]
        fxns = self.fxns2plot[1:]

        # THIS IS DESIGNED FOR PLOTTING ALL COLS OF DATA WITH OLD INDVARS FUNCTIONS
        # var = [float(x) for x in var]
        # fxns = [float(x) for x in fxns]
```


Figure 13: Plotting Class python code

```
226         for fn in fxns:
227             y_0 = [float(x) for x in self.data[fn]]
228             # x_0 =
229             m, b = np.polyfit(var,y_0,1)
230             x = np.linspace(min(var), max(var), num=len(var))
231             y = m * x + b
232             txt1 = "LinReg line for y = " + self.dataLabels[fn]
233             txt2 = "and x = " + self.dataLabels[var]
234             txt3 = "y = (%.4f" % m + ")x + (%.4f" % b + ")"
235             txt4 = "R^2 = %.4f" % ChEplot.rSquared(var, y_0)
236             print( f"{txt1:<35}{txt2:<30}{txt3:>20}{txt4:>20}")
237             if self.dataColors is None:
238                 self.figure.axis[0].plot(x, y, \
239                     linewidth=width ,linestyle=style)
240             else:
241                 self.figure.axis[0].plot(x, y, \
242                     color=self.dataColors[fn], \
243                     linewidth=width ,linestyle=style)
244 
245     # def calc(self):
246     #   pass
247 
248     # def plotErrorBars(self):
249     #   x = self.data(self.fxns2plot[0])
250     #   for y in self.fxns2plot[1:]:
251 
252 
253     #Statistics
254     @staticmethod
255     def rSquared(x, y):
256         x = x.reshape((-1,1))
257         y_reg = LinearRegression().fit(x,y)
258         return y_reg.score(x,y)
259 
260     def printAllRSquared(self, precision=5, vars=None, fxns=None):
261         if vars is None:
262             vars = range(0, self.numDataSets)
263         if fxns is None:
264             fxns = range(0, self.numDataSets)
265 
266         for fn in fxns:
267             for var in vars:
268                 if fn == var:
269                     continue
270                 rSquared = ChEplot.rSquared(self.data[0],self.data[fn])
271                 rStr = "R^2 = %1." + str(precision) + "f"
272                 rStr = rStr % rSquared
273                 if rStr is None: print("Error_0")
274                 if self.dataLabels is None: print("Error_1")
275                 print( f"{rStr:<25}{self.dataLabels[fn-self.numDataVars]:<20}{'with
    respect to':<20}{self.dataLabels[var]:>10}")
276 
277     #COMPLETE ME
278     def confInterv(self, n=1):
279         self.lowerBound_CI = []
280         self.upperBound_CI = []
281         for fn in range(self.numDataVars, self.numDataSets):
282             x_bar , stdDev = np.mean(self.data[fn]) ,np.std(self.data[fn])
```


Figure 14: Plotting Class python code

```
283             SE = stdDev / math.sqrt(self.num)
284             DoF = n
285             stats.t.ppf(q=0.05,)
286             scipy.stats.t.ppf(q=.05,df=22)
287
288
289     #Plot: Setters
290     def setFxns2Plot(self, fxns):
291         self.fxns2plot = fxns
292
293     def setDataStyles(self, styles: list):
294         self.lineStyles = styles
295
296     def setDataColors(self, colors=None):
297         #Assign Random Colors, if no custom color array is given
298         if colors == None:
299             colors = []
300             for i in range (len(self.data)):
301                 color = "#"+''.join([random.choice('0123456789ABCDEF') for j in range(6)
302                 colors.append(color)
303
304         self.dataColors = colors
305         self.setLRegLineColors(colors)
306
307     def setAxisLabels(self, x: str, y:str, indepVar=0, xpadding=5, ypadding=5):
308         self.figure.axis[indepVar].set_xlabel(x,labelpad=xpadding)
309         self.figure.axis[indepVar].set_ylabel(y,labelpad=ypadding)
310
311     def setTicProps(self, _size=4, _width=1, _direction='in'):
312         self.figure.axis[0].xaxis.set_tick_params(which='major', size=_size, width=_widt
    direction=_direction, top='on')
313         self.figure.axis[0].xaxis.set_tick_params(which='minor', size=_size, width=_widt
    direction=_direction, top='on')
314         self.figure.axis[0].yaxis.set_tick_params(which='major', size=_size, width=_widt
    direction=_direction, right='on')
315         self.figure.axis[0].yaxis.set_tick_params(which='minor', size=_size, width=_widt
    direction=_direction, right='on')
316
317     def setNumTics(self, delta_x=0.1, delta_y=0.1, x_subTics=3, y_subTics=3):
318         self.figure.axis[0].xaxis.set_major_locator(mpl.ticker.MultipleLocator(delta_x))
319
    self.figure.axis[0].xaxis.set_minor_locator(mpl.ticker.MultipleLocator(delta_x/x_subTics
320         self.figure.axis[0].yaxis.set_major_locator(mpl.ticker.MultipleLocator(delta_y))
321
    self.figure.axis[0].yaxis.set_minor_locator(mpl.ticker.MultipleLocator(delta_y/y_subTics
322
323     #Plot: Features
324     def showLegend(self, x=0.01, y=0.01, width=1, height=1, _loc='lower left',
    frame=True,_fontSize=10):
325         # plt.legend(bbox_to_anchor=(x,y, width, height), loc=_loc, frameon=frame,
    fontsize=_fontSize)
326         plt.legend(frameon=frame, fontsize=_fontSize)
327
328
329     def changeFont(self, font='Alvenir', size=10, linewidth=0.9):
330         mpl.rcParams['font.family'] = font
331         plt.rcParams['font.size'] = size
332         plt.rcParams['axes.linewidth'] = linewidth
333
```


Figure 15: Plotting Class python code

```
334     #Presentation
335     def showPlot(self):
336         "Shows the figure"
337         plt.show()
338 
339     #Save
340     def savePlot(self, filename="poop.png", _dpi=900, _transparent=False,
_bbox_inches='tight'):
341         "Saves the Figure(graph) made to a file"
342         plt.savefig(filename, dpi=_dpi, transparent=_transparent,
bbox_inches=_bbox_inches)
343 
344     #Close the figure, plots, and data associated with the object
345     def close(self):
346         "Close the figure(window) that we were plotting in"
347         plt.close(self.figure)
```


Figure 16: Plotting Class python code