Lab Rapport 1

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2023

Abstract

We did two experiments, in the first experiment where we did measurements on resonance frequency of 5 different gases. In the second experiment we conducted molecular dynamics simulations. By fitting a model to the data in experiment 1 we where able to experimentally find the speed of sound in the different gases. We compared these findings with the theoretical values and found that all percentage errors where below 7%. Thus, we could argue based on the results assuming ideal gas is a reasonable assumption.

We then did molecular dynamics simulations showing that this assumption became worse with increasing density, but we managed to simulate only a 0.25% deviation from the ideal gas simulating a low characteristic density $\rho^* = 0.001$.

1 Introduction

In two experiments we explore the attributes of gasses using two experimental settting. The first is using sound waves and 5 different gases and states to gain insight into the ideal gas model. In the second experiment we conduct a molecular simulation and use the results from this part to our experimental observations.

In the first experiment we use a tube which we filled with 5 different gases and states. In the tube we use accoustics to find the resonance frequency of the gas, by using a oscilliscope. We test the frequencies ranging from 200Hz to 2kHz and note the resonance frequencies we observe in the oscilliscope. We then conduct a linear regression and find the slope, the use this to find the speed of sound in gas. We are working under the assumption that diatomic gasses have 5 quadratic degrees of freedom, three translational and two rotational. Whereas, monoatomic gasses only have tre degrees of translational freedom. Thus we are essentially interested in exploring how this assumption performs by comparing the speed of sound calculated from theoretical and experimental values.

In the second experiment we use the LAMMPs molecular dynamics program where do explore various charachteristics of a gas. We find heat capacity from the simulation and use it determine the degrees of freedom in the gas molecules. Furthermore, we make the simlation more advanced by looking at Nitrogen gas where we compare the results with findings from the first experiment.

2 Methods

2.1 Experiments using sound waves

2.1.1 Finding frequencies

We use a oscilliscope to find the resonance frequencies corresponding the gas of interest inside the tube. We manually look for the frequencies by changing the frequency of the oscilliscope and visually look for the maximum amplitude. We start to look for resonance frequencies starting with 200Hz and slowly increasing the frequency to 2kHz as we look for the resonance frequencies along the way.

We use this method for 5 experimental settings. We start first by looking at air at room temperature. Second we look at Argon, third CO2, fourth was heated air at a temperature 45 °C, and lastly air at 66 °C.

We write a script (see code 1) that fits a linear regression to the experimental data. Furthermore, it outputs the relevant values: speed of sound in the gas $c[m/s]$, the theoretical value c_{theory}, the standard error, the slope $a[1/s]$.

We find the theoretical speed of sound using the following formula:

$$c = \sqrt{\frac{(f+2)RT}{fM_{mol}}} \tag{1}$$

Where f is the quadratic degrees of freedom. For all experiments wee assume the gas to have 5 degrees of freedom. R is the universal gas constant $8.31[J/molK]$, M_{mol} is the molar mass of the specific gasses in Kg/mol, with the different gases having the following values: Air - $28.97g/mol$; Argon - $39.489g/mol$; CO2 - $44g/mol$. T is the temperature in kelvins. However, T is calculated using the omic resistance of the thermic resistor in the tube, using the following equation,

$$T_C \approx 25 - 24ln(r) + 274 \tag{2}$$

Where, $r = R/(10^5)$, where R is the ohmic resistance of the thermistor (Dysthe, 2023, p.17).

For the uncertainty of the fit to our experimental data we use the following general formula for uncertainty (Dysthe, 2023, p.22), using the following formula,

$$\delta c = c\sqrt{\left(\frac{\delta a}{a}\right)^2 + \left(\frac{\delta L}{L}\right)^2} \tag{3}$$

Where, δa is found from the slope of our linear regression fit, essentially using the standard error from the fit. L is the length of the tube given as $1243mm$ and its measurement uncertainty is given as $\delta L = 1.5mm$

2.2 Molecular dynamics simulations

2.2.1 Simulating the experimental conditions

For the molecular dynamic experiment we use LAMMMPs to run simulation on the Lennard-Jones system. We read the logfiles and calculate the heat-capacity C_V and the partition function Z. We find it using the relation $Z = \frac{P}{\rho T}$, where P, ρ and T is the pressure , mass density and temperature resulting from the LAMMPs simulation. We derive the degrees of freedom from the definition of heat capacity at constant volume,

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{V,N} \tag{4}$$

We solve (4) using U from the equipartition relation $\frac{U}{N} = \frac{f}{2}kT$. Which results in

$$C_V = \frac{f}{2}Nk \tag{5}$$

In order to find the heat capacity C_V we find the slope of a linear fit to the data, as we did in experiment 1.

We run the simulation my modifying some of the conditions. First, we change the temperature and observe the results. By using this knowledge we go on to simulate Nitrogen gas and compare the results on the degrees of freedom with our experimental findings.

3 Results

3.1 Experiments using sound waves

The results for the gas experiments are as following and the experiments corresponding datavalues.

3.1.1 Gas: Air

Figure 1 is the resulting linear fit, figure 2 is the raw measured values and figure 3 is the metrics from the calculations. We can see from the table figure 3 that we measured speed of sound in Air 319.04 ± 0.19

3.1.2 Gas: Heated Air

For the heated air the results was as following, figure 4 is the resulting linear fit, figure 5 is the raw measured values and figure 6 is the metrics from the calculations. We can see from the table figure 6 that we measured speed of sound in Air at 45 celsius degrees. 374.52 ± 0.10.

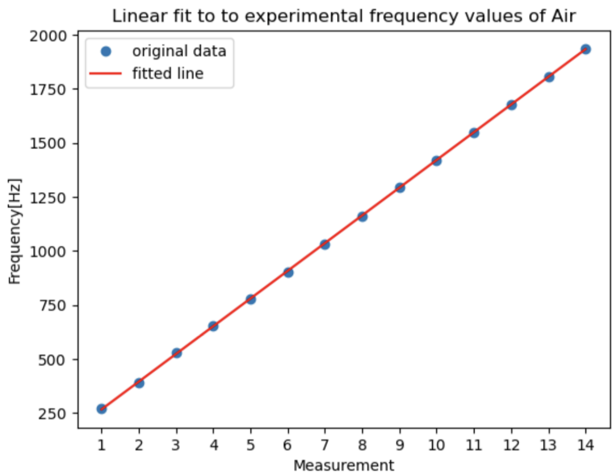

Figure 1: Linear fit for air at room temperature.

Measurement nr	Measured frequencies[Hz]
1	270.5
2	389.5
3	527.5
4	651.5
5	779.5
6	904.5
7	1033.5
8	1161.5
9	1292.5
10	1420.5
11	1548.5
12	1678.5
13	1807.5
14	1936.6,

Figure 2: Table containing the measured values for air at room temperature..

3.1.3 Gas: Heated Air 2

For the heated air 2 the results was as following, figure 7 is the resulting linear fit, figure 8 is the raw measured values and figure 9 is the metrics from the calculations. We can see from the table figure 6 that we measured speed of sound in Air at 66 celsius degrees. 359.87 ± 0.24.

3.1.4 Gas: Argon

For the Argon gas the results was as following, figure 10 is the resulting linear fit, figure 11 is the raw measured values and figure 12 is the metrics from

Metric	Value
Speed of sound[m/s]	319.040
Theoretical c	369.670
Percentage error between theory and experiment	13.696
Standard error	0.192
Our experimental value of a[Hz]	128.335
Uncertainity of speed of sound c	0.613)

Figure 3: Table containing the metrics from the calculations for air at room temperature..

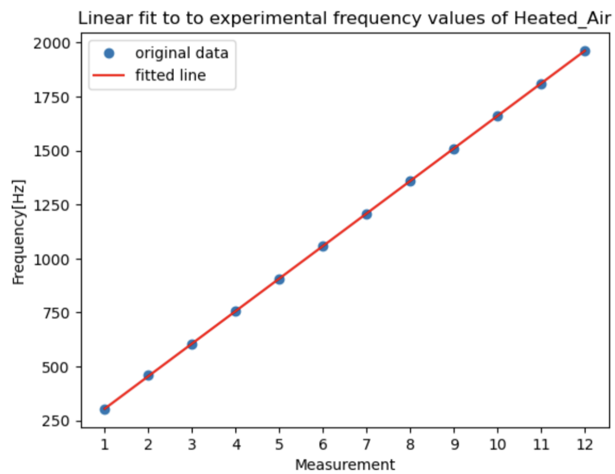

Figure 4: Linear fit for heated air at 45 celcius degrees.

the calculations. We can see from the table figure 12 that we measured speed of sound in Argon at celsius degrees. 319.14 ± 0.11.

3.1.5 Gas: CO2

For the CO2 gas the results was as following, figure 13 is the resulting linear fit, figure 14 is the raw measured values and figure 15 is the metrics from the calculations.We can see from the table figure 15 that we measured speed of sound in CO2 at 262.97 ± 1.7.

Measurement nr	Measured frequencies[Hz]
1	303.2
2	458.5
3	606.5
4	756.3
5	906.2
6	1057.3
7	1207.7
8	1358.8
9	1510.1
10	1660.8
11	1811.4
12	1962.6,

Figure 5: Table containing the measure values for heated air at 45 celcius degrees.

Metric	Value
Speed of sound[m/s]	374.524
Theoretical c	369.670
Percentage error between theory and experiment	1.313
Standard error	0.105
Our experimental value of a[Hz]	150.653
Uncertainity of speed of sound c	0.522)

Figure 6: Table containing the metrics from the calculations for heated air at 45 celcius degrees.

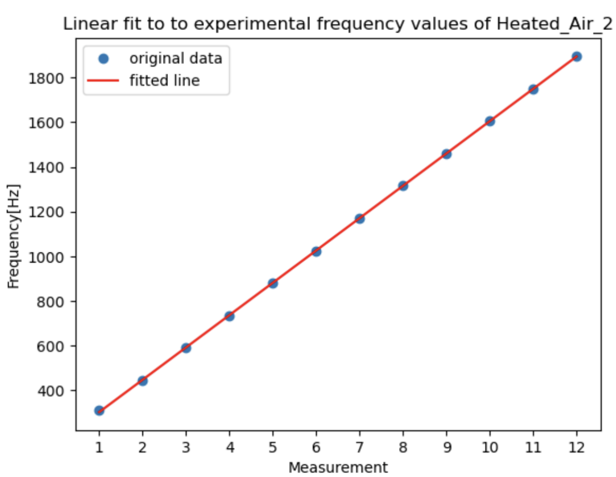

Figure 7: Linear fit for heated air at 66 celcius degrees.

Measurement nr	Measured frequencies[Hz]
1	309.1
2	446.0
3	589.2
4	734.1
5	879.3
6	1023.1
7	1168.1
8	1315.5
9	1459.6
10	1605.4
11	1751.1
12	1896.5,

Figure 8: Table containing the measure values for heated air at 66 celcius degrees.

Metric	Value
Speed of sound[m/s]	359.877
Theoretical c	358.066
Percentage error between theory and experiment	0.506
Standard error	0.243
Our experimental value of a[Hz]	144.762
Uncertainity of speed of sound c	0.745)

Figure 9: Table containing the metrics from the calculations for heated air at 66 celcius degrees.

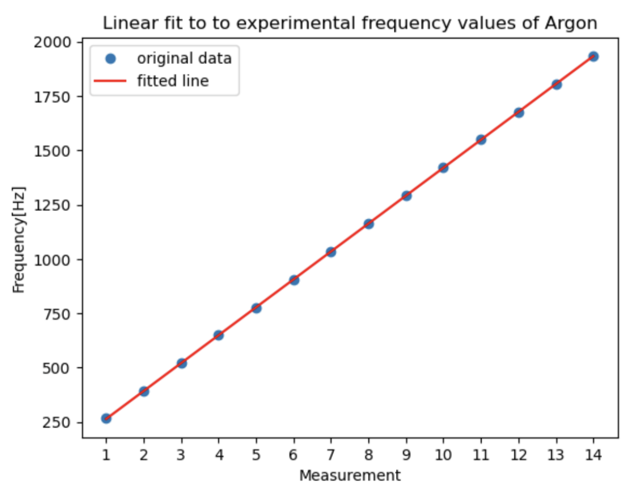

Figure 10: Linear fit for argon.

Measurement nr	Measured frequencies[Hz]
1	268.5
2	391.0
3	519.8
4	649.2
5	777.8
6	903.1
7	1032.8
8	1162.3
9	1291.4
10	1419.6
11	1548.6
12	1675.4
13	1805.5
14	1934.1,

Figure 11: Table containing the measure values for argon.

	Metric	Value
0	Speed of sound[m/s]	319.147
1	Theoretical c	322.242
2	Percentage error between theory and experiment	0.960
3	Standard error	0.116
4	Our experimental value of a[Hz]	128.378
5	Uncertainity of speed of sound c	0.482)

Figure 12: Table containing the metrics from the calculations for argon.

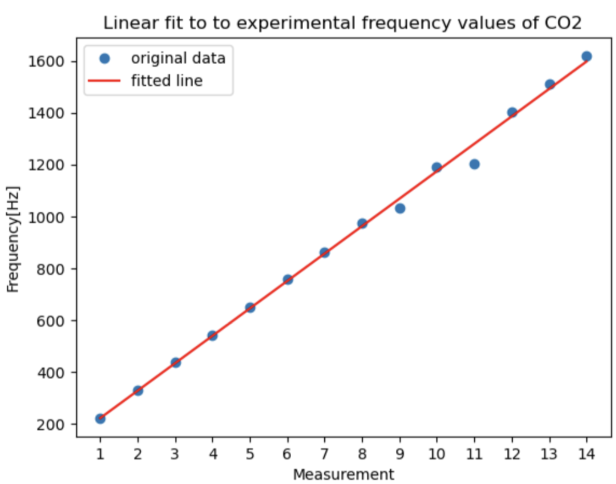

Figure 13: Linear fit for CO2.

Measurement nr	Measured frequencies[Hz]
1	222.8
2	329.9
3	435.9
4	540.6
5	649.9
6	757.5
7	863.9
8	972.3
9	1030.6
10	1188.5
11	1204.1
12	1402.4
13	1512.9
14	1619.3,

Figure 14: Table containing the measure values for CO2.

Metric	Value
Speed of sound[m/s]	262.976
Theoretical c	279.791
Percentage error between theory and experiment	6.010
Standard error	1.798
Our experimental value of a[Hz]	105.783
Uncertainity of speed of sound c	4.480)

Figure 15: Table containing the metrics from the calculations for CO2.

3.2 Molecular dynamics simulations

3.2.1 Simulation 1

Using $\rho^* = 0.001$ and initial temperature $T_0^* = 1$ we have plotted both U^* and Z as functions of the temperature T^* respectively in figure 16 and figure 17. Using (5) we found

$$C_v = (1.4962 \pm 0.0005)\ J/K$$

and

$$\bar{Z} = (0.996 \pm 0.009)$$

.

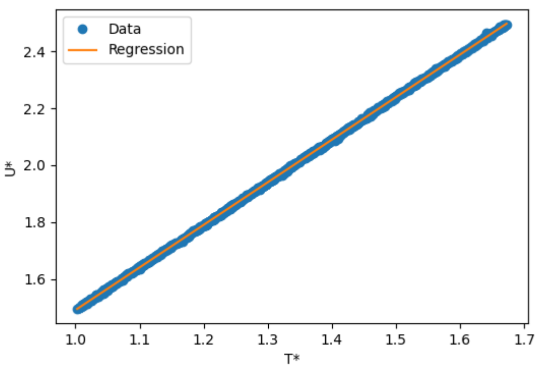

Figure 16: The characteristic thermal energy U^* as a function of the characteristic time for the first Lennard-Jones simulation.

3.2.2 Simulation 2

Furthermore we ran the same simulation only changing the temperature, it went from the triple point temperature $T^* = 0.69$ to 10 times the critical temperature $T^* = 1.32$. $U^*(T^*)$ is plotted in figure 18 and $Z(T^*)$ is plotted in figure 19. Both values are very similar at

$$C_V = (149730 \pm 4) \cdot 10^5\ J/K$$

and

$$\bar{Z} = (0.999 \pm 0.005)$$

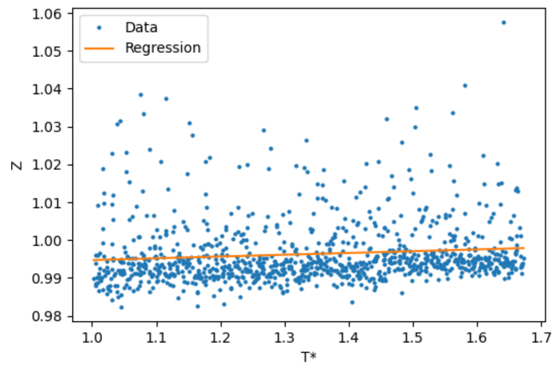

Figure 17: The compressibility factor Z as a function of the characteristic time for the first Lennard-Jones simulation. We see that it is almost constant $Z \approx 1$.

3.2.3 Simulation 3

We used the following ten different ρ^*-values ranging from easy gas density up to close to the triple point ($\rho^* = 0.85$) at temperature $T^* = 1.4$

$$\rho^* = [0.001, 0.1, 0.18, 0.28,$$
$$0.38, 0.47, 0.57, 0.66, 0.75, 0.84]$$

All the heat capacities C_V are plotted in figure 20. Figure 21 plots Z as a function of ρ^*, and figure 22 plots $C_V(\rho^*)$.

3.2.4 Simulation 4

For the rodmodel we got

$$C_V = (1.262 \pm 0.02)\ J/K$$

and

$$f = (2.524 \pm 0.003)$$

For the spring model we got

$$C_V = (1.734 \pm 0.008)\ J/K$$

and

$$f = (3.51 \pm 0.02)$$

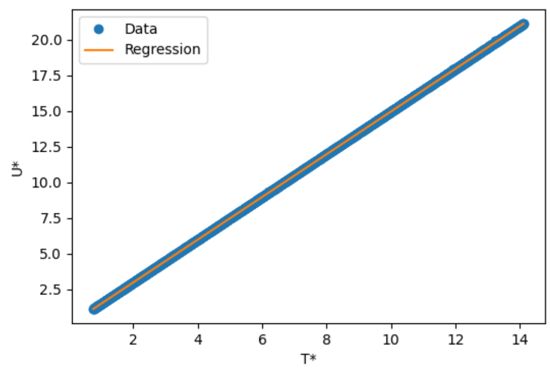

Figure 18: The characteristic thermal energy U^* as a function of the characteristic time for the second Lennard-Jones simulation.

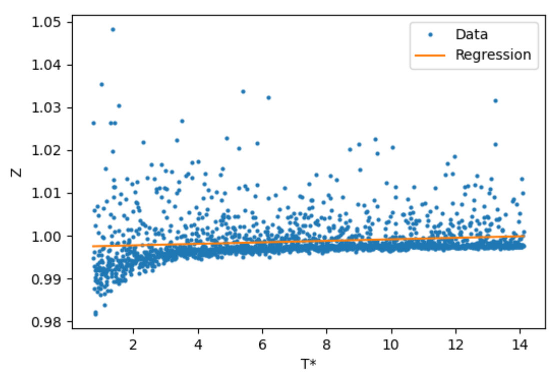

Figure 19: The compressibility factor Z as a function of the characteristic time for the second Lennard-Jones simulation. Again we see $Z \approx 1$.

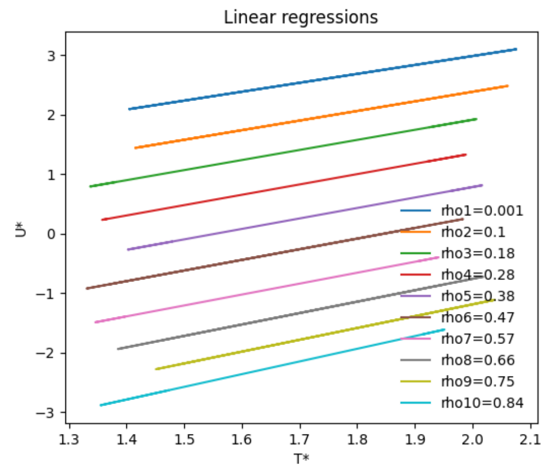

Figure 20: The characteristic thermal energy U^* as a function of the characteristic time for third Lennard-Jones simulation, plotted with ten different characteristic densities.

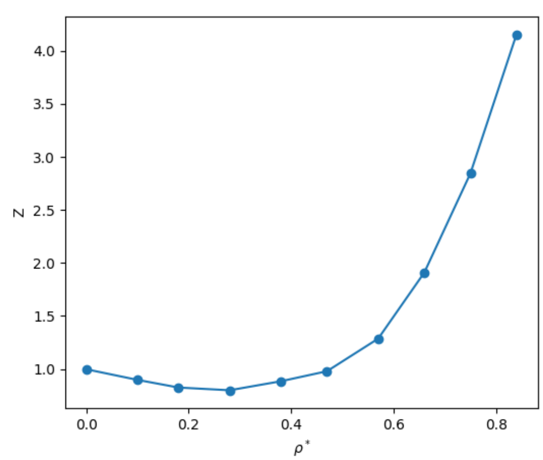

Figure 21: The compressibility factor Z as a function of the characteristic density for the third Lennard-Jones simulation.

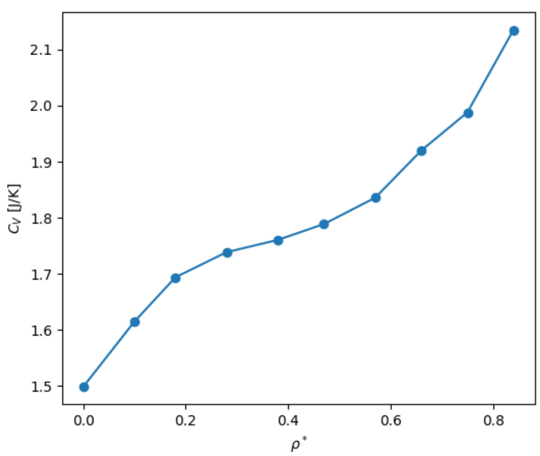

Figure 22: The heat capacity C_V as a function of the characteristic density the third Lennard-Jones simulation.

4 Discussion

4.1 Experiments using sound waves

The first observation from the metric calculations of the 5 different gas conditions is that the theoretical calculation of the speed of sound is nearly identical to the experimental findings. All measurements have a below 7% error from the theoretical value. The air that had the highest temperature was the least different from expected theoretical value. Thus, an interesting observation of the air gases in different temperatures was that the hotter the air the less the error is between expected from theory and experimental. However, as the change in degrees of freedom does not occur for the temperatures we were working with this difference migth not be caused by temperature, but possibly to the fact that all 3 air gas measurements were conducted on three different setups. Thus this may have been caused by different setups.

It is also important to note that the uncertainty does not encompass this finding. Nevertheless, the overall result considering the relatively small percentage errors between theoretical expectation and experimental findings - we can argue that 5 degrees of freedom for diatomic molecules and 3 for monoatomic molecules is probably a reasonable assumption that we worked under. Thus we can say that the underlying assumption of an ideal gas, is an reasonable assumption to use for describing the behavior of gases, at least of the conditions of these experiements considering not extreme temperature.

4.2 Molecular dynamics simulations

4.2.1 Simulation 1

For an ideal gas we expect $Z = 1$ and from (5) with $f = 3$ degrees of freedom (and $N = k = 1$) we expect $C_V = 3/2 = 1.5$. We used $f = 3$ because this simulation simulates a mon-atomic gas with only translational degrees of freedom. Our simulated Z-factor was within the uncertainty of the ideal gas' factor, and C_V had only a 0.25% relative difference which we are happy with.

4.2.2 Simulation 2

Both the heat capacity C_V and the compressibility factor Z were very similar, only slightly changing with the temperature. C_V only deviated 0.07% from the previous simulation and $\bar{Z}$ deviated 0.30%. The both are still approximately equal to the ideal gas values.

4.2.3 Simulation 3

We can clearly both see the C_V and Z changing with changing density, much more than with temperature. They both are moving more and more away from the ideal gas values. This makes sense considering the ideal gas has no inter-particle interactions, and a higher and higher density will provide more and more particle interactions.

4.2.4 Simulation 4

In the experiments we derived that N_2 gas will have five degrees of freedom at around room temperatures, three translational and two rotational, so we see the spring model simulation is more accurate on this front. They both have very similar deviations from the ideal gas C_V, the rod and spring model respectively deviate 15.87% and 15.60%.

References

D. K. Dysthe, Vetle A. Vikenes, C.A. Lutken and A. L. Read (2023). FYS2160 Lab1: Gas thermodynamics. Univserity of Oslo.

A Appendix: Code

```
from scipy.stats import linregress
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

frequencies_Air = [270.5, 389.5, 527.5,
    651.5, 779.5, 904.5, 1033.5, 1161.5,
    1292.5, 1420.5, 1548.5, 1678.5, 1807.5,
    1936.6]
```

```python
frequencies_Ar = [268.5, 391.0, 519.8, 649.2, 777.8, 903.1, 1032.8, 1162.3, 1291.4, 1419.6, 1548.6, 1675.4, 1805.5, 1934.1]
frequencies_CO2 = [222.8, 329.9, 435.9, 540.6, 649.9, 757.5, 863.9, 972.3, 1030.6, 1188.5, 1204.1, 1402.4, 1512.9, 1619.3]
frequencies_Heated_Air = [303.2, 458.5, 606.5, 756.3, 906.2, 1057.3, 1207.7, 1358.8, 1510.1, 1660.8, 1811.4, 1962.6]
frequencies_Heated_Air_2 = [309.1, 446.0, 589.2, 734.1, 879.3, 1023.1, 1168.1, 1315.5, 1459.6, 1605.4, 1751.1, 1896.5]

def theory_c(M_mol_gas, f, resistance_val):
    R = 8.31
    T_in_K = 25 - 24*np.log(resistance_val*10**3/10**5) + 274
    Theoretical_c = np.sqrt((f+2)*R*T_in_K/(f*M_mol_gas))
    return Theoretical_c

def gas_diagnostic(frequencies, gas_name, M_mol_gas, f, resistance_val):

    x = np.arange(1, len(frequencies)+1)

    df = {"Measurement nr": x, "Measured frequencies[Hz]":frequencies,
         }
    full_tbl = pd.DataFrame(df)
    res = linregress(x, frequencies)
    plt.plot(x, frequencies, 'o', label='original data')
    plt.plot(x, res.intercept + res.slope*x, 'r', label='fitted line')
    plt.xticks(x)

    L = 1243/1000
    delta_L = 1.5/1000
    c = res.slope*2*1.243
    delta_a = res.stderr
    a = res.slope
    uncertainity = c*np.sqrt((delta_a/a)**2 + (delta_L/L)**2)
    #print("Uncertainity of speed of sound c:", uncertainity)

    #print("---------------------")
    #print(full_tbl)
    print("-----------------------")
    print("Speed of sound[m/s]:", np.round(res.slope*2*L, decimals=3))
    print("Theoretical c:", np.round(theory_c(M_mol_gas, f, resistance_val), decimals=3))
    print("Percentage error between theory and experiment:", np.round(np.abs((theory_c(M_mol_gas, f, resistance_val) - res.slope*2*L)/theory_c(M_mol_gas, f, resistance_val))*100, decimals=3), "%")
    print("Standard error:", np.round(res.stderr, decimals=3))
    print("Our experimental value of a[Hz]:", np.round(res.slope, decimals=3))
    print("Uncertainity of speed of sound c:", np.round(uncertainity, decimals=3))
    print("--------------------")
    plt.title(f"Linear fit to experimental frequency values of {gas_name}")
    plt.ylabel("Frequency[Hz]")
    plt.xlabel("Measurement")
    plt.legend()
    plt.show()

    df = {"Measurement nr": x, "Measured frequencies[Hz]":frequencies,
         }
    full_tbl = pd.DataFrame(df)


    df_metrics = {"Metric":["Speed of sound[m/s]", "Theoretical c", "Percentage error between theory and experiment", "Standard error",
                          "Our experimental value of a[Hz]", "Uncertainity of speed of sound c"],
                  "Value":[np.round(res.slope*2*L, decimals=3), np.round(theory_c(M_mol_gas, f, resistance_val), decimals=3), np.round(np.abs((theory_c(M_mol_gas, f, resistance_val) - res.slope*2*L)/theory_c(M_mol_gas, f, resistance_val))*100, decimals=3), np.round(res.stderr, decimals=3), np.round(res.slope, decimals=3), np.round(uncertainity, decimals=3)]
                 }

    metric_tbl = pd.DataFrame(df_metrics)

    return full_tbl, metric_tbl
```

Listing 1: Code used for experiment 1

```python
"""
Created on 25.09.2023
"""

from sys import argv

import lammps_logfile as lmplog
import matplotlib.pyplot as plt
```

```python
import numpy as np
from scipy.stats import linregress

if __name__ == "__main__":
    # Constants
    rho = 0.001

    log = lmplog.File(argv[1])

    # Extract values
    T = log.get("Temp")[1:]
    U = log.get("TotEng")[1:]
    P = log.get("Press")[1:]

    # Regression
    reg = linregress(T, U)
    y = reg.slope * T + reg.intercept

    # Plot
    figsize = (6, 4)
    plt.figure(figsize=figsize)
    plt.plot(T, U, "o", label="Data")
    plt.plot(T, y, label="Regression")
    plt.legend()
    plt.xlabel("T*")
    plt.ylabel("U*")
    plt.savefig("U(T).png")

    def mean_std(array):
        return np.mean(array), np.std(array)


    # Calculate values
    Cv = reg.slope
    dCv = reg.stderr

    f = Cv * 2
    df = f * dCv / Cv

    Z_arr = P / (rho * T)
    Z, dZ = mean_std(Z_arr)

    # Plot Z:
    reg_Z = linregress(T, Z_arr)
    y_Z = reg_Z.slope * T + reg_Z.intercept
    plt.figure(figsize=figsize)
    plt.plot(T, Z_arr, "o", label="Data", ms=2)
    plt.plot(T, y_Z, label="Regression", ms=2)
    plt.legend()
    plt.xlabel("T*")
    plt.ylabel("Z")
    plt.savefig("Z(T).png")

    # Save prints to output file
    with open("analyze.txt", "w") as file:
        file.write(f"C_v = ({Cv:.7f}    {dCv:.7f})\n")
        file.write(f"f = ({f:.7f}    {df:.7f})\n")
        file.write(f"Z_mean = ({Z:.7f}    {dZ:.7f})\n")
```

Listing 2: Code used for analyzing seperate lammps simulations

```python
"""
Created on 25.09.2023
"""

import lammps_logfile as lmplog
import numpy as np
import matplotlib.pyplot as plt

from pathlib import Path
from scipy.stats import linregress

path = Path(".")

# List of outfiles
outfiles = list(path.rglob("log.task3_rho*"))
# Put second item (rho10) to the back for correct loop indexing
outfiles.append(outfiles.pop(1))

# List of density values
rho_vals = np.genfromtxt("task3_infiles/rho_vals.txt")

Z_vals = np.zeros(len(rho_vals))
Cv_vals = np.zeros_like(Z_vals)

# Analyze each one, then plot Cv(T) and Z(rho)
# First plot Cv(t)
figsize = (6, 5)
plt.figure(figsize=figsize)
i = 0
for file, rho in zip(outfiles, rho_vals):
    log = lmplog.File(file)

    # Extract values
    T = log.get("Temp")[1:]
    U = log.get("TotEng")[1:]
    P = log.get("Press")[1:]

    # Regression
    reg = linregress(T, U)
    y = reg.slope * T + reg.intercept

    # Plot U regression
    rho_index = file.name.split("_")[-1]
```

```python
    plt.plot(T, y, label=f"{rho_index}={rho}", ms=2)

    # Save mean Z values
    Z_vals[i] = np.mean(P / (rho * T))

    # Save C_v (slope) values
    Cv_vals[i] = reg.slope

    i += 1

plt.legend(frameon=False)
plt.xlabel("T*")
plt.ylabel("U*")
plt.title("Linear regressions")
plt.savefig("U(T).png")

# Secondly, plot Z(rho)
plt.figure(figsize=figsize)
plt.plot(rho_vals, Z_vals, "o-")
plt.xlabel(r"$\rho^*$")
plt.ylabel("Z")
plt.savefig("Z(rho).png")

# Lastly plot C_V(rho)
plt.figure(figsize=figsize)
plt.plot(rho_vals, Cv_vals, "o-")
plt.xlabel(r"$\rho^*$")
plt.ylabel("$C_V$ [J/K]")
plt.savefig("C_V(rho).png")
```

Listing 3: Code used for analyzing multiple lammps simulations in task 3.