Quantifying Temperatures Effect on Hydrogen Storage Capacity Of Metal Hydride

By. Jessica Arnoldi

Research Background

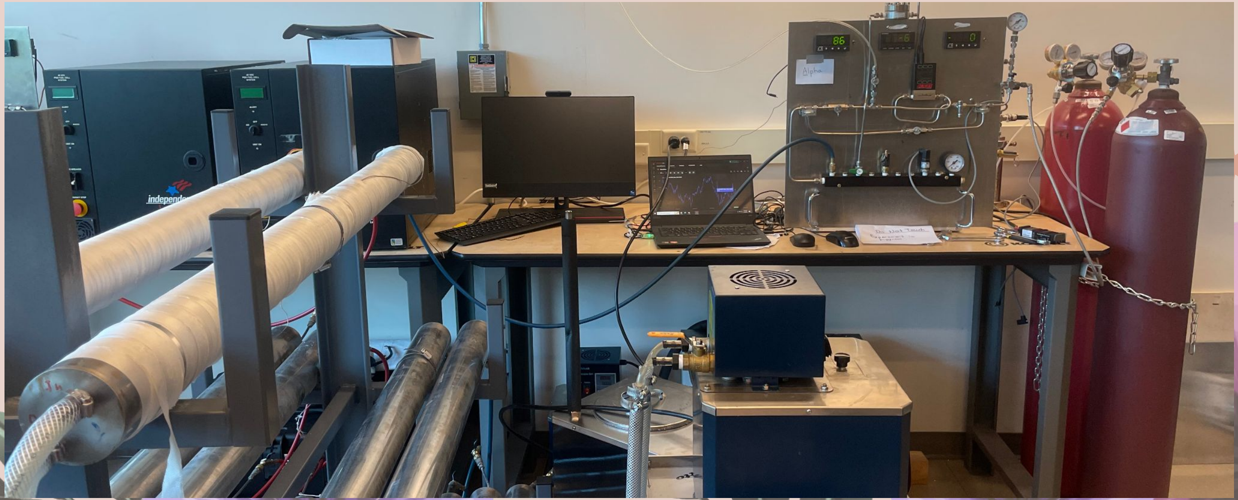
Recent focus is on replacing natural gas with hydrogen to achieve complete decarbonization of power and transportation sectors by 2050.

Hydrogen has been shown to be a clean and effective energy carrier with the potential to be a long-term renewable energy resource. However, it is envisioned that blended hydrogen in natural gas is a likely scenario during this transition.

The main issue with Hydrogen is the storage. A potential solution is solid-state metal hydride storage.

Current research is focusing on characterizing the effects of entry pressure, temperature, and flowrate on total hydrogen storage capacity.

This portion of the study focuses on the effect of temperature while pressure and flowrate are kept stable at 50 psi and 20 SLPM respectively.



Problem

- The minimum time of a test is several hours resulting in over 8000 data points
- Often multiple tests are required to obtain an averaged data set
- Due to the type of data collected calculations are difficult using excel
- Graphing is problematic due to the number of data points and incorporating several tests on the same graphs even more so

Goal

- Have code that can take in and separate the generated data from a CSV file and change the flow from SLPM to SLPS
- Integrate under the flow rate curve to obtain the total volume of gas adsorbed for each temperature
- Plot both the Mass Flow vs. Time and Total Mass vs. Time
- Plot the total mass for each temperature in a bar graph to illustrate how temperature affects storage volume.
- Determine approximately how long it takes for the volume adsorbed to reach equilibrium or 90% of the total volume for each temperature.

Coding Approach

Importing Data

```python
#main imports
from numpy import*
import pandas as pd
import scipy as sp
import matplotlib.pyplot as plt
```

```python
#use the Pandas library to read the data
datafile_20 = pd.read_csv('04-14 50 PSI 20 SLPM 20 C .csv')

#create arrays with the Mass Flow data
MF_20=array([datafile_20['MASSFLOW']])
#convert the Mass Flow from SLPM to SLPS ()
MF_20=MF_20/60

#flaten MF_20 so it has the same dimension that linspace will create
MF_20=MF_20.flatten()
```

Integrating Data

```
#set x values
L=MF_20.size
X=linspace(0,L,L)

#integrate under the curve to obtain the Total Mass
Int_20=sp.integrate.cumulative_trapezoid(MF_20,X)
#isolate the total mass
TM_20=Int_20[-1]
```

Plotting The Mass Flow

```
#create a plot of the Mass Flow over Time
plt.plot(X,MF_20,'gold')
plt.ylabel('Mass Flow (SLPS)')
plt.xlabel('Time (Seconds)')
plt.title('Mass Flow vs. Time 20˚C')
plt.show()
```

Plotting The Integral

```
#create a plot of the Total Mass over Time
plt.plot(X[1:],Int_20,'orange')
plt.ylabel('Total Mass (Liters)')
plt.xlabel('Time (Seconds)')
plt.title('Total Mass vs. Time at 20˚C')
plt.show()
```

```
print('The total mass is approximately {:.2f} L at 20˚C'.format(TM_20))
```

Integrating Data

```
print('The total mass is approximately {:.2f} L at 20˚C'.format(TM_20))
```

```
#Math to calculate how long it takes to reach equalibrium approx. 90% of total mass
eq=.9*TM_20
#find the position of eq in TM
above_eq=where(Int_20>=eq)
eq_pos=above_eq[0][0]
#convert from seconds
eq_T_20=eq_pos/60
eq_T_20_h=eq_T_20/60
print('Equalibrium occures after approximately {:.2f} min or {:.2f} hours at 20˚C'.format(eq_T_20,eq_T_20_h))
```

```
#calculating an approximate error on the total mass (this is due to the integration method)
#this portion could be expanded to average multiple tests at a single temperature for increased accuracy
err_20=TM_20*.1
err_20_T=eq_T_20_h*.1
```

Plotting Total Mass

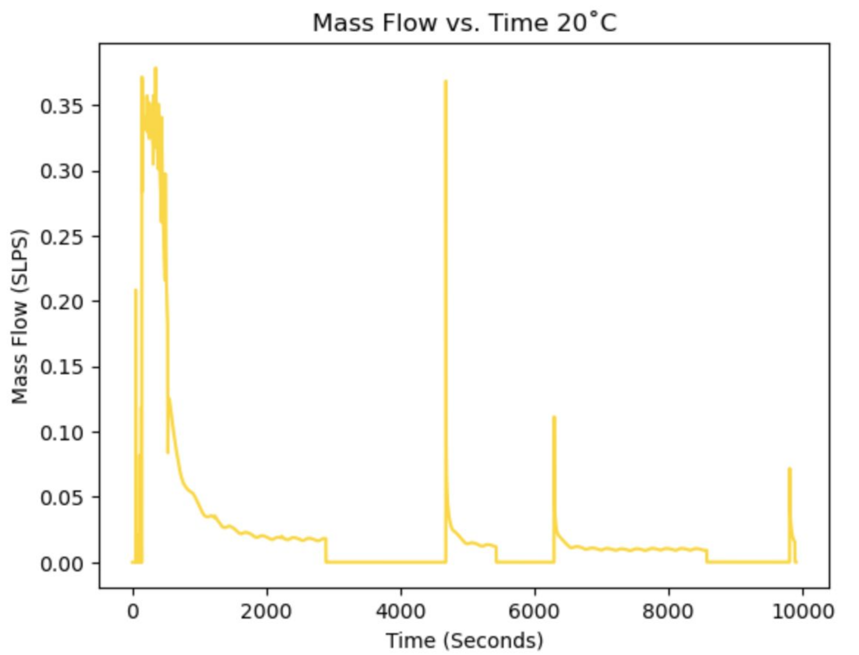
```
#graph the total mass at each temperature with error bars in a bar graph
plt.bar('20˚C',TM_20,yerr=err_20,alpha=.5,ecolor='darkorchid',capsize=10,color='orange')
plt.bar('10˚C',TM_10,yerr=err_10,alpha=.5,ecolor='darkorchid',capsize=10,color='limegreen')
plt.bar('5˚C',TM_5,yerr=err_5,alpha=.5,ecolor='darkorchid',capsize=10,color='cornflowerblue')
plt.ylabel('Total Mass (Liters)')
plt.xlabel('Temperature')
plt.title('Total Mass vs. Temperature')
plt.show()
```

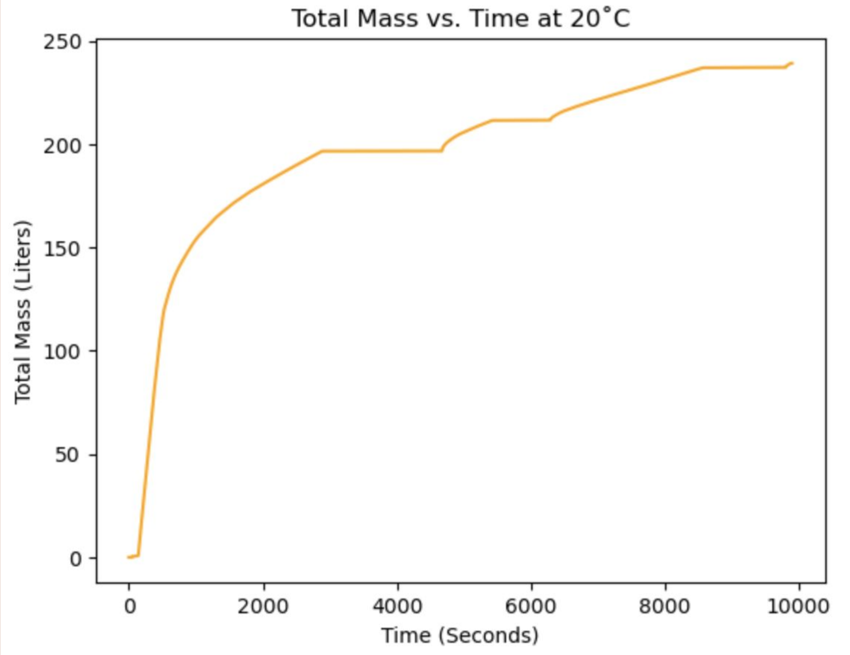
Plotting Equilibrium Time

```
#graph the total mass at each temperature with error bars in a bar graph
plt.bar('20˚C',eq_T_20_h,yerr=err_20_T,alpha=.5,ecolor='darkorchid',capsize=10,color='orange')
plt.bar('10˚C',eq_T_10_h,yerr=err_10_T,alpha=.5,ecolor='darkorchid',capsize=10,color='limegreen')
plt.bar('5˚C',eq_T_5_h,yerr=err_5_T,alpha=.5,ecolor='darkorchid',capsize=10,color='cornflowerblue')
plt.ylabel('Equalibrium Time (Hours)')
plt.xlabel('Temperature')
plt.title('Equalibrium Time vs. Temperature')
plt.show()
```

Results & Discussion

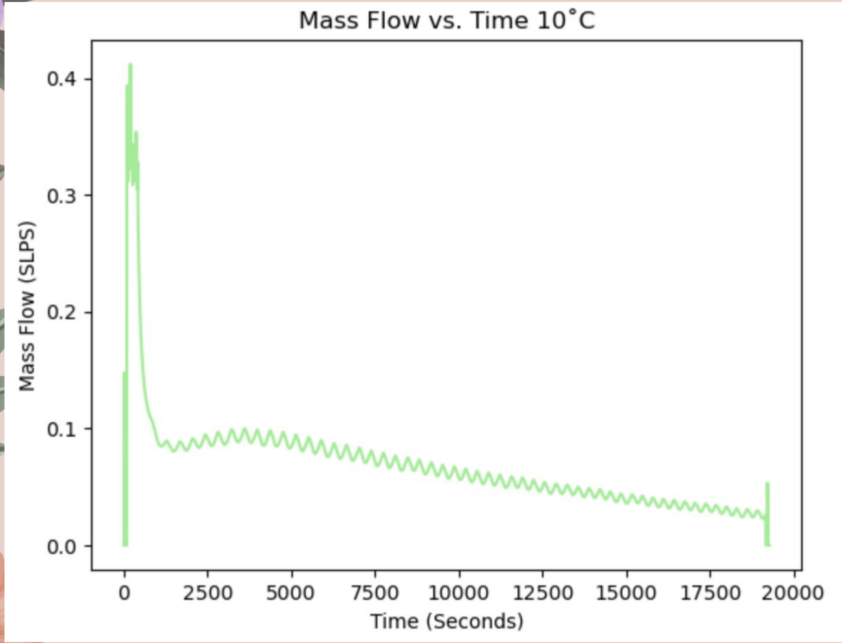
Results 20˚C

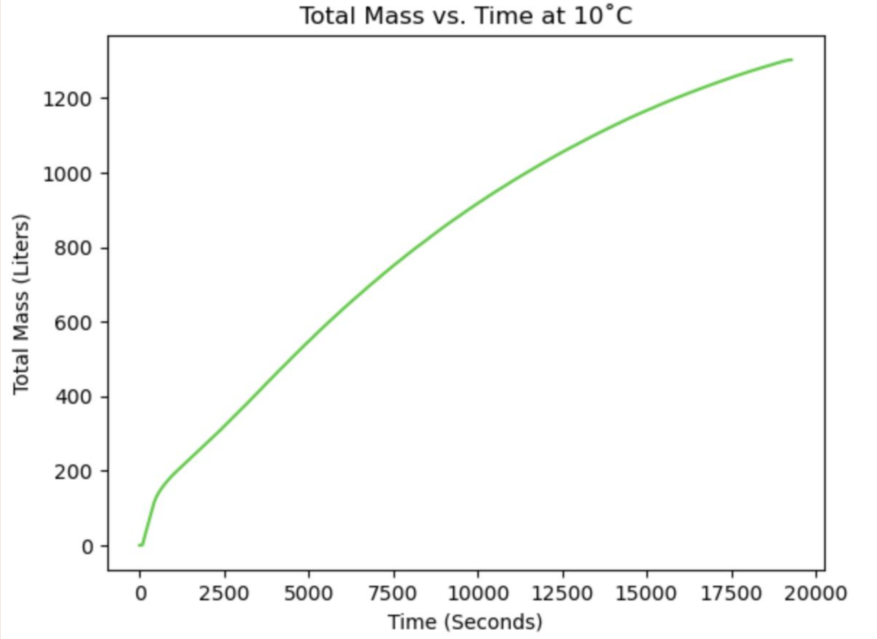





```
The total mass is approximately 239.14 L at 20˚C
Equalibrium occures after approximately 107.27 min or 1.79 hours at 20˚C
```

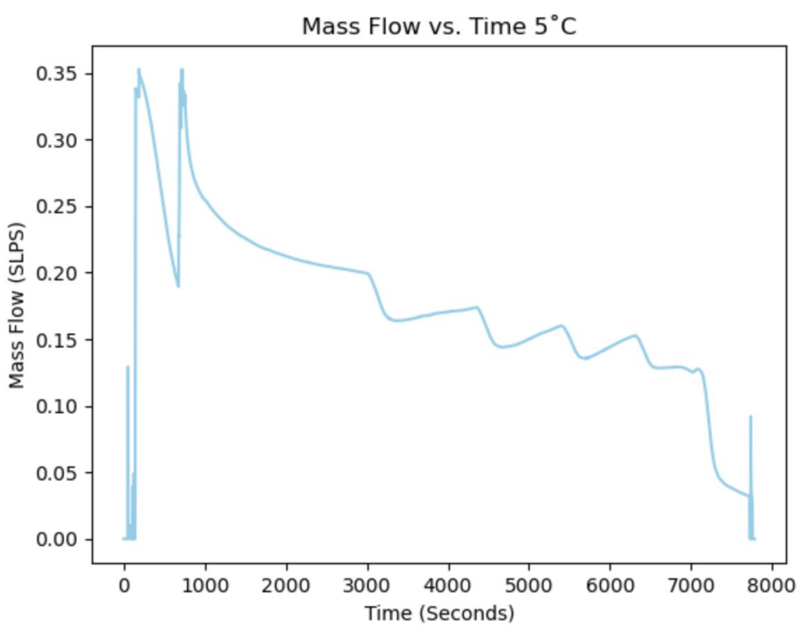
Results 10˚C

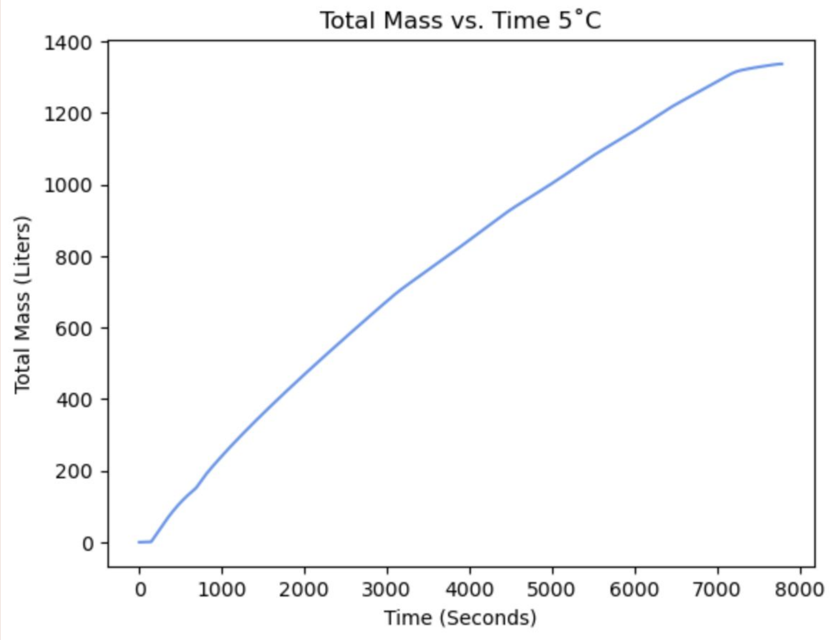




The total mass is approximately 1302.88 L at 10˚C
Equalibrium occures after approximately 252.52 min or 4.21 hours at 10˚C

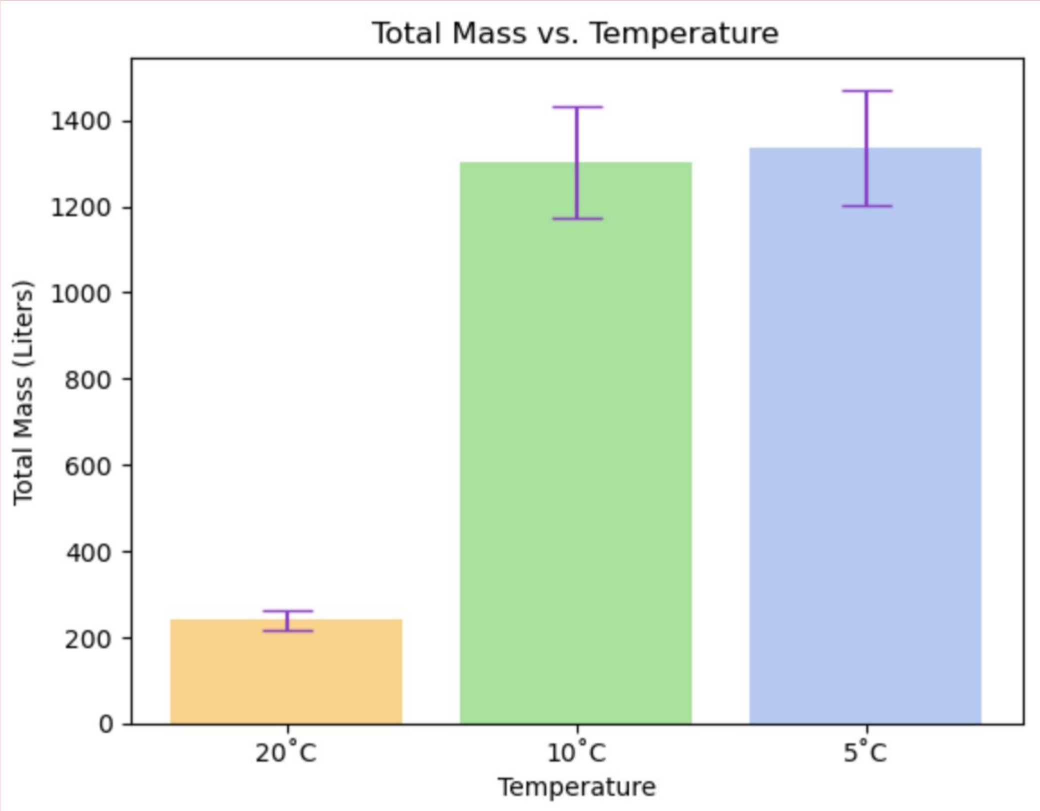
Results 5°C



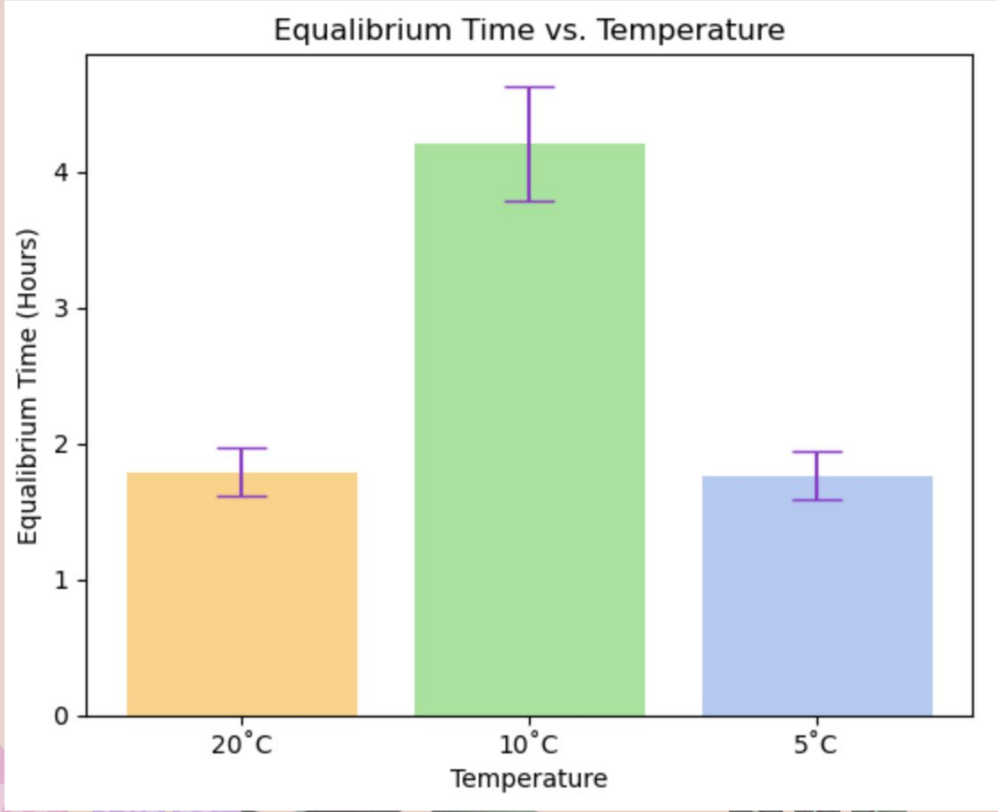


The total mass is approximately 1337.28 L at 5˚C
Equalibrium occures after approximately 105.87 min or 1.76 hours at 5˚C

Total Mass Comparison



Equilibrium Time Comparison



Conclusions

- The temperature had a significant effect on the total storage capacity. However, after 10°C the effect appears to plateau.
- Time required to reach equilibrium appears to peak at 10°C rather than increase proportionally with total stored mass.
- According to the Mass Flow vs. Time graph it appears the the target flow rate of 20 SLPM is only maintained for approximately the first 30 minutes of testing.

Future Work

- The goal would eventually be to have multiple tests for each temperature and average the data for a more accurate result.
- Having multiple datapoint would also allow for the use of standard deviation error instead of fixed estimates
- Since the eventual goal is to store/transport Hydrogen at room temperature another analysis rout would be quantifying the pressure rise from adsorption temperature to room temperature