

# ps5\_ipynb

November 5, 2025

```
[11]: # put data into lists; for each row of applied potential, we have current at
      ↪different times
      ''
      \begin{center}
      \begin{tabular}{l/l/l/l/l/l/l/l/l}
      \hline
      Current in $\mu \mathrm{m} \ \mathrm{A} / \ \mathrm{cm}^2$ & \multicolumn{6}{|c|}{Time}
      ↪elapsed after step, $s$} \\
      \hline
      Applied Potential, $V$ & 0.1 & 0.2 & 0.5 & 0.9 & 1.4 & 2.5 \\
      \hline
      -0.60 & 0.18 & 0.13 & 0.08 & 0.06 & 0.05 & 0.04 \\
      \hline
      -0.55 & 1.3 & 0.84 & 0.53 & 0.41 & 0.32 & 0.26 \\
      \hline
      -0.50 & 8.5 & 6.2 & 4.0 & 2.9 & 2.4 & 1.8 \\
      \hline
      -0.45 & 57.6 & 42.2 & 26.9 & 19.3 & 15.4 & 11.8 \\
      \hline
      -0.40 & 324 & 233 & 143 & 106 & 88 & 64 \\
      \hline
      -0.35 & 958 & 651 & 422 & 312 & 260 & 179 \\
      \hline
      -0.30 & 1307 & 874 & 565 & 435 & 339 & 254 \\
      \hline
      -0.25 & 1358 & 1009 & 596 & 453 & 355 & 275 \\
      \hline
      -0.20 & 1369 & 951 & 588 & 461 & 377 & 275 \\
      \hline
      -0.15 & 1394 & 980 & 602 & 459 & 367 & 276 \\
      \hline
      -0.10 & 1375 & 969 & 618 & 452 & 353 & 271 \\
      \hline
      -0.05 & 1376 & 979 & 623 & 446 & 368 & 260 \\
      \hline
      0.00 & 1345 & 946 & 606 & 460 & 359 & 280 \\
      \hline
      
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\end{tabular}
\end{center}
'''

import numpy as np
import matplotlib.pyplot as plt

data_dict = {
    '-0.60': [0.18, 0.13, 0.08, 0.06, 0.05, 0.04],
    '-0.55': [1.3, 0.84, 0.53, 0.41, 0.32, 0.26],
    '-0.50': [8.5, 6.2, 4.0, 2.9, 2.4, 1.8],
    '-0.45': [57.6, 42.2, 26.9, 19.3, 15.4, 11.8],
    '-0.40': [324, 233, 143, 106, 88, 64],
    '-0.35': [958, 651, 422, 312, 260, 179],
    '-0.30': [1307, 874, 565, 435, 339, 254],
    '-0.25': [1358, 1009, 596, 453, 355, 275],
    '-0.20': [1369, 951, 588, 461, 377, 275],
    '-0.15': [1394, 980, 602, 459, 367, 276],
    '-0.10': [1375, 969, 618, 452, 353, 271],
    '-0.05': [1376, 979, 623, 446, 368, 260],
    '0.00': [1345, 946, 606, 460, 359, 280],
}

# Convert to numpy arrays
voltages = np.array([float(v) for v in data_dict.keys()])
currents_array = np.array([data_dict[v] for v in data_dict.keys()]) # Shape: (13, 6)
times = np.array([0.1, 0.2, 0.5, 0.9, 1.4, 2.5]) # Time points in seconds

R = 8.314 # J/(mol K)
T = 298 # K
n = 1 # number of electrons transferred
F = 96485 # C/mol
t = 0.1 # seconds
C = 1

# Now you can plot using the arrays
plt.figure()
currents_1d = currents_array[:,0]
# plot E ≈ E^0 + \frac{RT}{nF} \ln \left( \frac{C}{i(t) \sqrt{t}} - 1 \right) to back out E^0
E0_values = voltages - (R * T) / (n * F) * np.log(C / (currents_1d * 1e-3 * np.sqrt(t)) - 1)
# do a scatter plot
plt.scatter(voltages, E0_values)
plt.xlabel('Applied Potential (V)')
plt.ylabel('Extracted E0 (V)')

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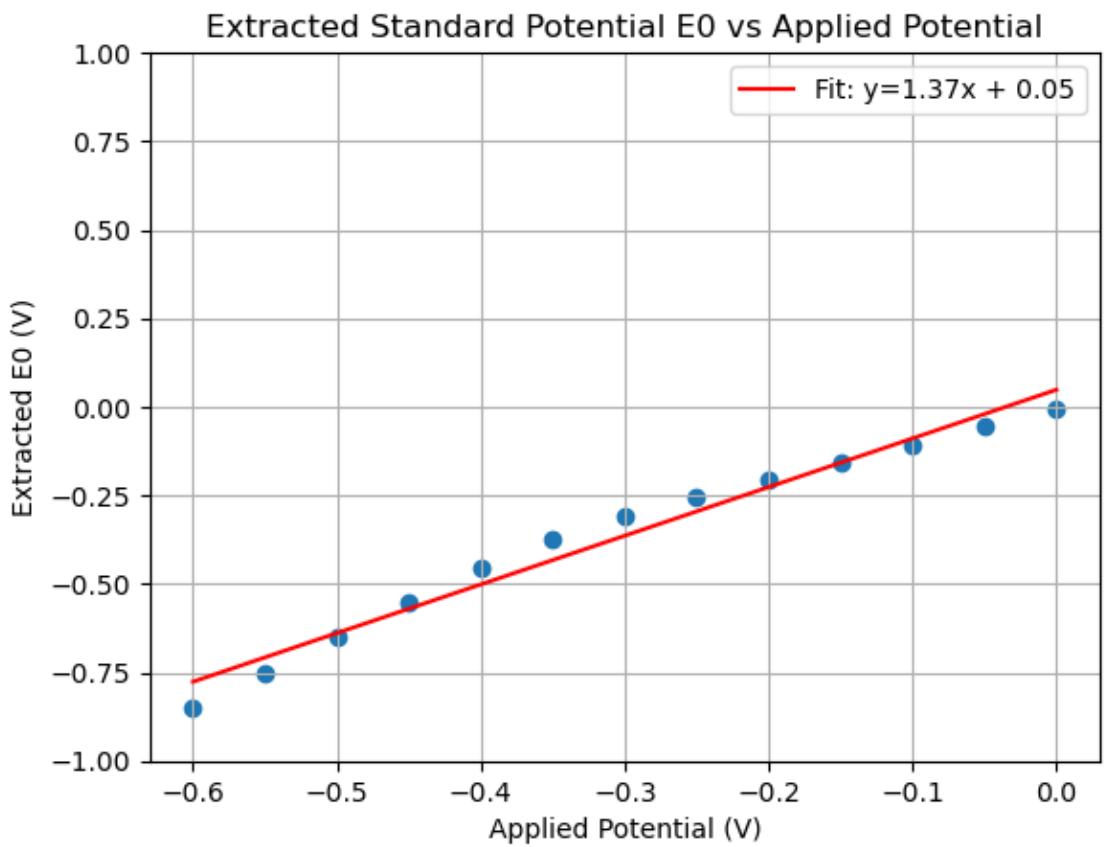
plt.ylim(-1,1)
# add a line of best fit
m1, b1 = np.polyfit(voltages, E0_values, 1)
plt.plot(voltages, m1 * voltages + b1, color='red', label=f'Fit: y={m1:.2f}x + {b1:.2f}')
plt.legend()
plt.title('Extracted Standard Potential E0 vs Applied Potential')
plt.grid()
plt.show()

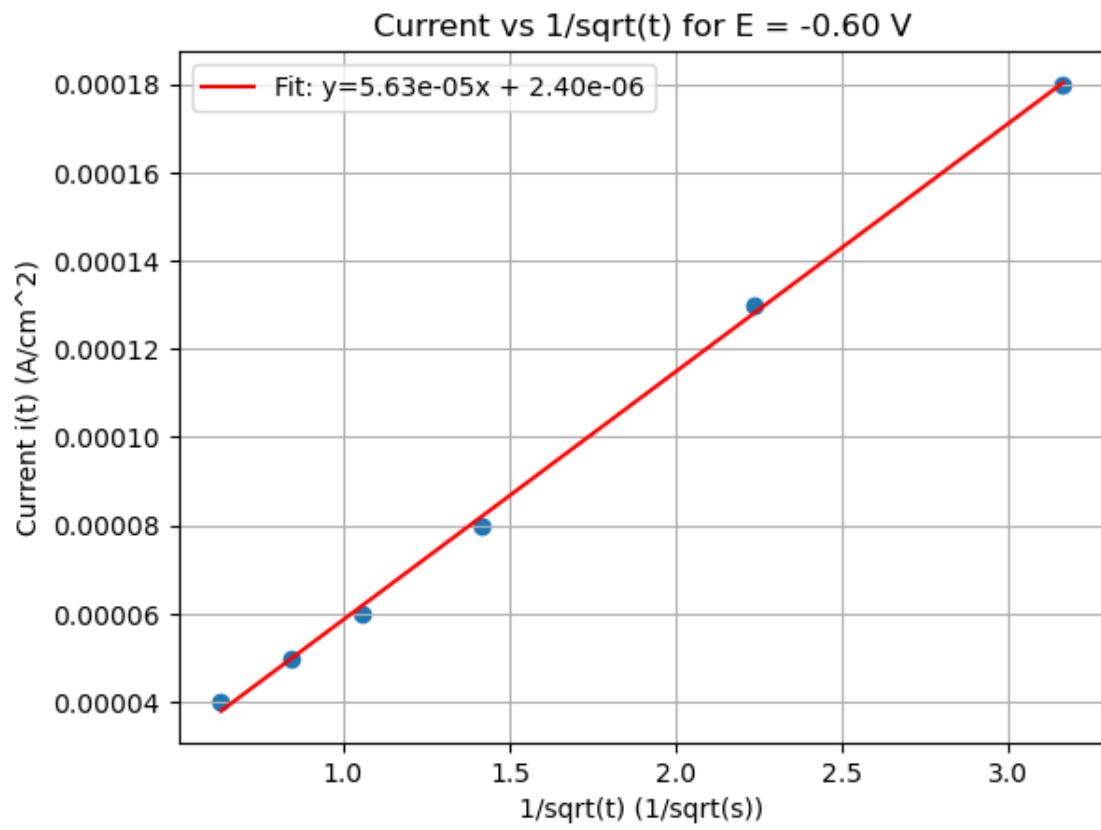
currents_1e = currents_array[0,:]
plt.figure()
# scatter plot i(t) vs 1/sqrt(t)
plt.scatter(1/np.sqrt(times), currents_1e * 1e-3) # convert to A/cm^2
plt.xlabel('1/sqrt(t) (1/sqrt(s))')
plt.ylabel('Current i(t) (A/cm^2)')
plt.title('Current vs 1/sqrt(t) for E = -0.60 V')
plt.grid()
# add a 1/sqrt(t) fit line
m2, b2 = np.polyfit(1/np.sqrt(times), currents_1e * 1e-3, 1)
plt.plot(1/np.sqrt(times), m2 * (1/np.sqrt(times)) + b2, color='red', label=f'Fit: y={m2:.2e}x + {b2:.2e}')
plt.legend()
plt.show()

#
$$C' \equiv \frac{\sqrt{D} F c_{\infty}^{*}}{(1+k) \sqrt{\pi}}$$
; back out D
c_0_star = 3e-6 # mol/cm^3
# 
$$\exp \left( \frac{nF}{RT} (E - E^{\infty}) \right) \equiv k(E)$$

k = np.exp((n * F) / (R * T) * (voltages[0] - b1)) # using first voltage and
# extracted E0
D = ((m2 * (1 + k) * np.sqrt(np.pi)) / (F * c_0_star))**2 # cm^2/s
print(f'Diffusion constant D: {D:.2e} cm^2/s')
print(m2/c_0_star)

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Diffusion constant D:  $1.19 \times 10^{-7}$   $\text{cm}^2/\text{s}$   
18.750392375972453

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