MEGN 570 – Final Project

Sarena Nguyen

Dr. Steven DeCaluwe

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Introduction

There is currently a copious amount of work being done in the renewable energy sector on both the research and industry side. The advancement of renewable energy generation technologies has led to the growth of the energy storage sector, which includes battery and fuel cell technologies. The electric vehicle industry has constantly strived to produce a battery that would be competitive with traditionally fueled vehicles. Theoretically, Li-air batteries have a potential energy density that can make electric vehicles a more viable option for all applications. At this current moment, this technology does not meet the potential. However, more research into various components, such as conductive binders or the carbon: catalyst: binder ratios, can speed up the growth. Theoretical models can also play a significant role in determining how various factors can aid the battery's performance.

In this document, a model constructed in both POLYMATH and Python will be studied. A one-dimensional particle model with analyze the effect of electrode microstructure, such as electrode volume fraction(*ε)*, on the discharge curve for the battery. The project will utilize concepts learned in the Electrochemical Systems Modeling course to analyze the performance of this battery.

Model Formulation

To model this system, various electrochemical equations were used. First, mass transfer equations and conservation equations were used to understand how the reactions occurred.

$$\frac{d(X_k)}{d(t)} = \left(\frac{1}{C_o}\right)\left(\frac{1}{\varepsilon}\right)\left(\frac{A_{Surf}}{A}\right)\left(\frac{1}{H_{elec}}\right)s_k$$

$$s_k = \frac{v_k}{nF}\, i_{far}$$

$$C_k = X_k C_o$$

The Butler-Volmer and current equations were also found to model the conservation of energy.

$$U = U_o + (T - T_o)\left(\frac{S_{rxn}}{nF}\right) - \left(\frac{RT}{nF}\right)\ln\left(a_k^{v_k}\right)$$

$$a_k = \gamma\left(\frac{C_k}{C_o}\right)$$

$$i_{far} = i_o \exp(-nF\beta RT\eta) - \exp\left(nF(1-\beta)RT\eta\right)$$

The following was used to model the chemical reaction parameters.

$$q_{rxn} = k_{rxn} C_{ac,A}^{a} C_{ac,B}^{b}$$

The cell thermodynamics equation was also included in the model.

$$\Delta G_{rxn} = \sum_{k} \nu_k \mu_k$$

$$u_k = u_k + z_k F \phi_k$$

All the inputs were derived from literature. A table with the values and the corresponding sources is provided below.

Variable	**Value**	**Source**
β	0.5	[2]
η	2.3 V	[3]
ε	0.01, 0.5, 0.99	-
n	4 moles	-
F	96,485 C/eq	-
R	8.314 J/molK	-
C_o	0.3 M	[4]
A_{surf}	2.57E-5 m^2	[5]
A	4.90E-12 m^3	[5]
H_{elec}	-16 kJ/mol	[6]
U_o	1.2 V	[5]
T	400 K	-
T_o	298 K	-
S_{rxn}	59 J/molK	[6]
ν_k	1	-
i_o	1 mA/cm^2	[1]

Results

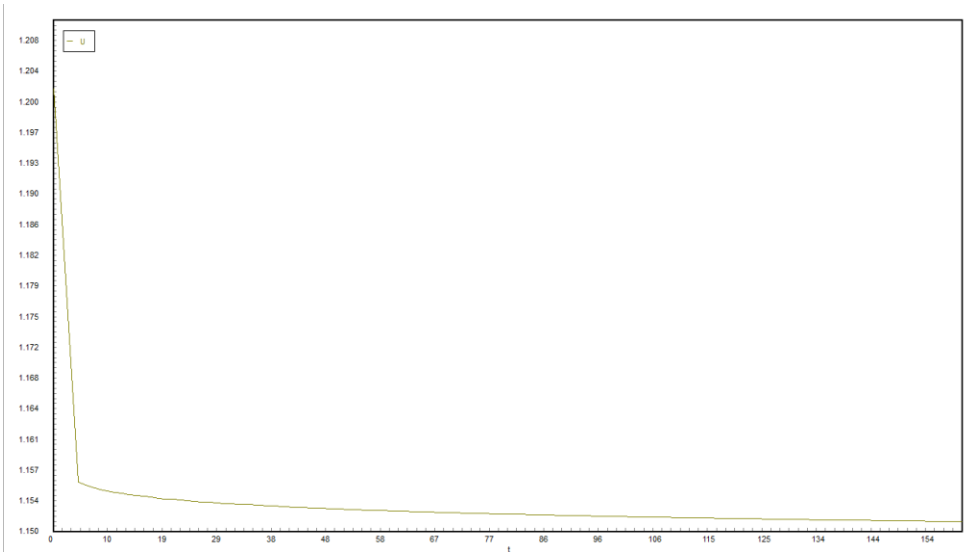

Figure 1: POLYMATH Discharge Curve ε= 0.1

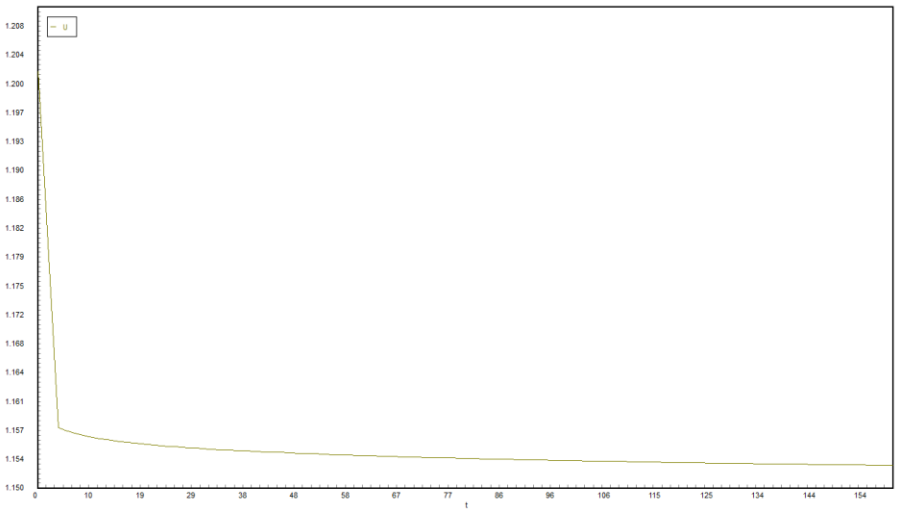

Figure 2: POLYMATH Discharge Curve ε= 0.5

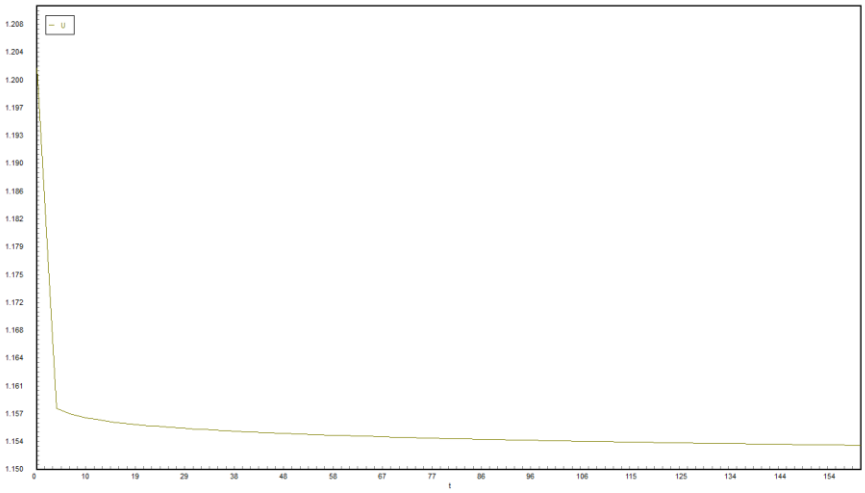

Figure 3: POLYMATH Discharge Curve ε= 0.99

Discussion

There were subtle differences between the discharge curves for different porosities. Three different porosity values were tested. First, the area where the curve started leveling out was set at a higher voltage for the higher porosity values. For *ε= 0.01,* the voltage was 1.161 V. For *ε= 0.99*, the voltage was set at 1.163 V. Furthermore, the voltage at the 160 second mark was higher for the higher values of porosity. However, there were fewer differences between the discharge curves for *ε= 0.50* and *ε= 0.99* compared to the *ε= 0.01*. The Python model was not able to generate any graphs, so POLYMATH was used.

Conclusions

All in all, the porosity values had a minor effect on the discharge curve for the Li-Air battery model. The voltage difference between the initial value and the value at the 160 second mark was greater for the lower porosity values. The curve plateaued at a higher voltage for the higher porosities and had a less significant drop over the 5 to 160 second mark. So, higher ε values produced a higher performing theoretical battery. Efforts were made to produce a model using Python programming methods. However, the model is still incomplete so a model in Polymath was used to produce results for further discussion. Future efforts will be made to review the model to find errors and to add additional parts to more closely model an experimental system.

Sources

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