MAE 298 Introduction to PDEs Electrochemical Modeling of Batteries

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Abstract—This

I. Introduction

PARTIAL differential equations (PDEs) provide a the mathematical basis for describing a significant number of scientific pheonimon; however, while the study of PDEs is import, it can often be more challenging to develope PDE which models these phenomina from first principles than it is to understand the structure of a given PDE. This can be more readily seen when investigating more complex systems which couple several PDEs together to describe the full dynamics of the system. To this point, electrochemical models of lithium-ion batteries fall into this category of complex systems. Even simple electrochemical models of batteries consist of anywhere upto five PDEs. The objective of this paper will be to derive the salient PDEs describing the electrochemical battery model known as Doyle-Fuller-Newman (DFN) model, with enough context and background about the first principles being applied to enlighten the reader as to how and why the given PDE model is meaningful.

II. Doyle-Fuller-Newman Model Overview

The DFN model has long been held as the gold standard electrochemical battery model. This model describes at the microscale dynamics of a planar battery cell (SHOWN IN FIG) which has been volume averaged to account for usage of this model as a full battery cell, which accounts for behaviors such as mass and charge conservation, as well as the process of intercalation and deintercalation where lithium is distributing through the material of electrode material or coating during charging and discharging respectively. This model can be broken down in to the five following categories. In turn, this paper will investigate each category, and provide the context and first principles analysis which yield appropriate governing PDEs.

1)
2)
3)
4)

III. Microscale Model Derivation

Before the complete Doyle-Fuller-Newman (DFN) model can be computed, it is neccessary to compute the microscale dynamics which govern the behavior of the compute electrochemical system. Only after this microscale model has been developed can we apply them to derving the complete DFN

model. In the microscale model, the principle mechanisms of operation are evaluated under the assumtion of homogeneous materials. Under this assumption, the model does not account for individual molecular interactions or impurities. For this analysis, we can assume that these molecular inconistentcies averaged out to create a homogeneous material for which we can independently derive and evaluate the governing equations for both the solid and electroyte phases of the battery.

A. Charge Conservation in Homogeneous Solid

The first step in this model is to use the principle of conservation of charge, in the solid phase of the battery. This means that charge is not created or destroyed within the battery. The principle used to derive this equation is the point for of **Ohms Law**. This means that we assume that through the electrode material, electron movement is caused by drifting of charge, as perscribed by Ohms Law. Namely...

$$\mathbf{i} = \sigma \mathbf{E}$$

Where $\mathbf{i}$ is the current density $[Am^{-2}]$, σ is the conductivity of the electrode material, and $\mathbf{E}$ is the applied electric field. This is an alternate form of Ohms Law ($V = IR$)

B. Mass Conservation in Homogeneous Solid

The conservation of mass in homogeneous solid (electrodes) is used to capture the dynamics of lithium intercalation into the crystalline structure of the electrode materials. Specifically, Fick's first law is used to describe quanity of molar flux density $\mathbf{N}$ to the gradient of lithium concentration in the solid electrode material, where D is the material dependent diffusivity.

$$\mathbf{N} = -D\nabla c$$

This expression states that the magnitude of the lithium molar flux density will increase with an increase in the gradient of the concentration. From this expression, we can compute the net molar flux by computing the integral of the entire domain boundary.

$$j = -\iint_S \mathbf{N} \cdot \hat{\mathbf{n}} dS$$

This is equivalent to the statement that ...

$$j = \frac{dn}{dt}$$

Where n is the number of moles. Furthermore, we can define dn as a function of concentration. This expression can be

computed by integrating each contribution of concentration within a differential volume over the entire volume of the domain.

$$dn = d \iiint_V c \, dV$$

By applying this substition and then and equating the net molar flux densities, we find that...

$$\iint_S \mathbf{N} \cdot \hat{n} \, dS = -\frac{d}{dt} \iiint_V c \, dV$$

This expression if the integral form of the continuity equation. The take away from this equation is that no mass has been created or destroyed inside the domain. Also this implies that all mass transfer which does occur happens only at the boundaries of the domain.

By further massaging and manipulating the previous equation, we can reduce this equation into the more familar form of Fick's second law, as shown below.

$$\frac{\partial c_S}{\partial t} = \nabla \cdot (D_S \nabla c_s)$$

The intuition behind this law is that it encapsulates the dynamic relationship between the concentration as it changes in time to the concentration as it changes in space.

C. Charge Conservation in Homogeneous Electrolyte

D. Mass Conservation in Homogeneous Electrolyte

E. Lithium Movement Between Solid & Electrolyte Phases

IV. DFN Model Derivation

V. Analysis of Governing Equations

VI. Numerical Solution

VII. Results

VIII. Conclusion

The conclusion goes here.

Acknowledgments

This should be a simple paragraph before the References to thank those individuals and institutions who have supported your work on this article.

IX. References Section

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X. Simple References

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References

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XI. Biography Section