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 lithiumion 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)

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

- B. Mass Conservation in Homogeneous Solid
- C. Charge Conservation in Homogeneous Electrolyte
- D. Mass Conservation in Homogeneous Electrolyte
- E. Lithium Movement Between Solid & Electrolyte Phases

III. DERIVATION

IV. Analysis of Governing PDEs

V. NUMERICAL SOLUTION

VI. RESULTS

VII. 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.

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