Simulation of drying process during fabrication of Lithium-Ion Battery porous electrode

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Introduction

Lithium Ion Battery Electrode Manufacturing Process

Mixing and Coating Unit Operations

Binder (B) eg: PVdF

Solvent (S) eg: NMP

PVdF-NMP Solution

Active Material (AM) eg: Graphite (MCMB)

Conductive Additive (CA)

Additional Solvent (S)

Mixing Unit Operation

Coating: drop casting

Mixed Slurry

Coating and Drying Unit Operations

Drying
Motivation

Life and Performance of cells

Mixing and Drying Process

- Solvent Evaporates
- Slurry (AM+B+CA+S)
- Metal Foil

Creates

Microstructure of Electrode

Affects

Porosity, Particle Distribution

Optimize Battery Electrode Manufacturing Process
Drying Phenomena

Drying happens in two Stages/Phases

Phase 1 - The coating dries at almost constant rate where solid consolidation (Shrinking of coating) happens and solvent evaporates.

Phase 2 - Evaporation continues beyond shrinking removing solvent from pores created.
Drying Model Development

Assumptions

➢ All solids (AM, B and CA) are treated together as single solid phase (Binder Migration is ignored).

➢ Shrinking happens only along the thickness direction (Area remains the same).

➢ Edge effects are ignored and drying along thickness direction is only considered.

➢ Temperature is constant (Oven is maintained at isothermal condition and sample size is small).

➢ Phase I is treated as saturated with liquid solvent.

➢ Effect of gravity is ignored.

➢ Gas phase is treated as a single component with both solvent vapour and dry air.
Mass Conservation of Liquid Solvent in Suspended Solid Medium

Momentum balance of Liquid Solvent in Suspended Solid Medium

Movement of Solid or Coating (Shrinking)
Drying Model Development

Model Geometry & Transport Phenomena

Phase 2

- Pores filled with vapour
- Pores filled with solvent (liquid)
- Solid

- Mass conservation of liquid solvent in porous medium
- Mass conservation of solvent in vapour phase in porous medium
- Momentum balance of solvent in porous medium
Governing Equations

Solvent Mass Conservation (liquid phase):

\[
\frac{\partial}{\partial t} (\rho_l \varepsilon_l) + \frac{\partial}{\partial t} (\rho_l \varepsilon_l u_l) = 0 \quad \text{(Phase 1)}
\]

\[
= -m \quad \text{(Phase 2)}
\]

Solvent Mass Conservation (Gas phase):

\[
\frac{\partial}{\partial t} (\rho_g \varepsilon_g) + \frac{\partial}{\partial t} (\rho_g \varepsilon_g u_g) = m \quad \text{(Phase 2)}
\]

Solvent Velocity:

\[
u_i = \frac{K \kappa_i}{\mu_l \varepsilon_i} \left( \frac{\partial P_i}{\partial x} \right); \quad i = l, g
\]

Coating Shrinking:

\[
u_s = - \frac{1}{A \rho_l} \frac{dw}{dt} \quad \text{(Phase 1)}
\]
<table>
<thead>
<tr>
<th>Transport Phenomena</th>
<th>Phase 1</th>
<th>Phase 2</th>
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<tr>
<td>Mass Conservation of liquid Phase:</td>
<td>General PDE</td>
<td>General PDE with Source term</td>
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<tr>
<td>Mass Conservation of Vapour Phase:</td>
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<td>Velocity of Liquid Phase:</td>
<td>Darcy’s Law</td>
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<tr>
<td>Velocity of Vapour Phase:</td>
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<td>Darcy’s Law</td>
</tr>
<tr>
<td>Velocity of Solid Phase (*)Coating thickness:</td>
<td>Moving Mesh</td>
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Case Study: Drying of Anode in Oven at 80 °C

Sample Experimental Parameters for Validation:

- Initial set thickness: 154 µm
- Area of coating: 23 cm²
- Total Solid content: 44 % of initial coating
- Initial weight of coating: 0.474 g
- Final porosity obtained before calendaring: 0.52
- Volume fraction of Solvent in the slurry: 0.72
Phase 1 (Shrinking of Electrode) Result comparison between model and Experiment

Model Predicts the stopping point of Shrinking accurately
Sample Validation Results

Result comparison between model and Experiment

Phase 2 of the model was stopped at 0.1 saturation

Comparison of Solvent evaporation predicted and measured
Future Extension

- Sedimentation of solid has to be included.
- Binder migration has to be included.
- Further refining of estimated mass and heat transfer coefficient from experiments has to be carried out.
- Accurate measurement of thickness is needed for better comparison.
- Parametric studies has to be carried out.
Acknowledgements

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