Battery Cell Electrochemical and Thermal Modeling

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Outline

- Battery **electrochemical** modeling using Simulor VHDL-AMS
- Battery cell **thermal** modeling using FLUENT
- From electrochemistry model to cell thermal model
Newman Pseudo 2d Electrochemistry Model

- Electrochemical Kinetics
- Solid-State Li Transport
- Electrolytic Li Transport

- Charge Conservation/Transport
- (Thermal) Energy Conservation

Lithium Ion Batteries

\[ \eta = (\phi_s - \phi_e) - U \]

\[ i_0 = k(c_e)^{a_2} (c_{s,max} - c_{s,e})^{a_2} (c_{e,s,e})^{a_1} \]

\[ \frac{\partial (\varepsilon c_e)}{\partial t} = \nabla \cdot (D_e \nabla c_e) + \frac{1 - t^+}{F} j^{Li} \]

\[ j^{Li} = a_s i_o \left\{ \exp \left[ \frac{\alpha_a F}{RT} \eta \right] - \exp \left[ - \frac{\alpha_c F}{RT} \eta \right] \right\} \]
What is VHDL-AMS

Very High Speed Integrated Circuit Hardware Description Language – Analog and Mixed-Signal

VHDL-AMS is a strict superset of IEEE Std. 1076
VHDL-AMS Model Construct

**Entity**
- Interface description of a subsystem or physical device
- Specifies input and output ports to the model

**Architecture**
- Behavior description
- Can be dataflow, structural, procedural, etc
- Modeling can deal with both analog (continuous) and digital (discrete) domains

[Diagram showing Entity and Architecture with input and output ports]
VHDL-AMS Model for a Capacitor

**Entity**

```
LIBRARY IEEE;
use IEEE.electrical_systems.ALL;
ENTITY cap IS
    GENERIC (
        capacitance : capacitance := 1.0e-3
    );
    PORT (
        QUANTITY init_v : IN voltage := 0.0;
        TERMINAL p : electrical;
        TERMINAL n : electrical
    );
END ENTITY cap;
```

The capacitor entity has one model constant, one input, and two terminals.

**Architecture**

```
ARCHITECTURE arch_cap OF cap IS
    QUANTITY voltage ACROSS current THROUGH p TO n;
    BEGIN
        IF (domain = quiescent_domain) USE
            voltage == init_v;
        ELSE
            current == capacitance * voltage'dot;
        END USE;
    END USE;
END ARCHITECTURE arch_cap;
```

The model description essentially has two lines, one for initial condition and one for the equation!!
VHDL-AMS Model for Heat Conduction

Example:

\[
\begin{align*}
\frac{\rho C_p}{k} \frac{\partial T}{\partial t} &= \frac{\partial^2 T}{\partial x^2} \\
T(x, 0) &= 20000x \quad x \in [0, 0.005] \\
T(x, 0) &= 20000(0.01 - x) \quad x \in [0, 0.01] \\
T(0.0, t) &= 0.0 \\
T(0.01, t) &= 0.0
\end{align*}
\]

- **Entity**

  ENTITY transient_diffusion IS
  generic
    
    \begin{align*}
    \text{rho: real} &= 2000.0; \\
    \text{k: real} &= 2.0; \\
    \text{Cp: real} &= 1000.0;
    \end{align*}
  END ENTITY transient_diffusion;

- **Architecture (main part)**

  IF (domain = quiescent_domain) USE
  \[
  \begin{align*}
  T_1 &= 20.0; \\
  T_2 &= 60.0; \\
  T_3 &= 100.0; \\
  T_4 &= 60.0; \\
  T_5 &= 20.0;
  \end{align*}
  \]

  ELSE
  \[
  \begin{align*}
  \text{rho*Cs*T1'} &= -(N1p - N0p)/h; \\
  \text{rho*Cs*T2'} &= -(N2p - N1p)/h; \\
  \text{rho*Cs*T3'} &= -(N3p - N2p)/h; \\
  \text{rho*Cs*T4'} &= -(N4p - N3p)/h; \\
  \text{rho*Cs*T5'} &= -(N5p - N4p)/h;
  \end{align*}
  \]

  END USE
VHDL-AMS Model for Electrochemistry

The governing equations of porous electrode model of the lithium-ion battery (Electrochemical Systems, 3rd by John Newman)

\[
\varepsilon \frac{\partial c}{\partial t} = \nabla \cdot (\varepsilon D \nabla c) - \frac{i_2 \cdot \nabla t^0}{z_+ \nu_+ F} + \frac{aj_n (1 - t^0)}{v_+} \\
i_2 = -\kappa \nabla \phi_2 + \frac{\kappa RT}{F} (1 - t^0) \nabla \ln c \\
I - i_2 = -\sigma \nabla \phi_1 \\
aF j_n = \nabla \cdot i_2 \\
j_n = i_0 \left\{ \exp \left( \frac{\alpha_a F}{RT} \eta_s \right) - \exp \left( -\frac{\alpha_c F}{RT} \eta_s \right) \right\}
\]

A coupled set of PDEs. The way to solve them with VHDL-AMS uses the same technique as before.
Model Implementation


\[ \phi_{1,1}, \phi_{1,2}, \phi_{1,3}, \phi_{1,4}, \phi_{1,5}, \phi_{1,6} \]

\[ i_{1,1}, i_{1,2}, i_{1,3}, i_{1,4}, i_{1,5}, i_{1,6} \]

\[ c_{1}, c_{2}, c_{3}, c_{4}, c_{5}, c_{6} \]

How to Use a VHDL-AMS Model in Simplorer?

• Drag and drop the VHDL-AMS model as if it is built-in.
• Double click to launch the property window as if it is built-in.
Newman Model – Dual Insertion

Simplorer’s Results

Newman’s Results

Newman Model – Temperature Impact

Concentration profiles due to different temperatures

Discharge curves due to different temperatures

Newman Model – Quantitative Comparison

Simplorer’s Results

White’s Results

Newman Model - Quantitative Comparison

Simplorer’s Results

White’s Results

Single Battery Cell Thermal Model

The model is based on the work of:

- Newman & Tidemann (1993);
- Gu (1983);
- Kim et al (2008)*

\[
\nabla \cdot (\sigma \nabla \phi) = J \quad \text{Transfer current}
\]

\[
J = Y (\phi_p - \phi_n - U) f(T)
\]

U and Y are derived from experimentally obtained polarization curve, dependent on Depth of Discharge (DOD) & Temperature

\[
U = a_0 + a_1(DOD) + a_2(DOD)^2 + a_3(DOD)^3
\]

\[
Y = a_4 + a_5(DOD) + a_6(DOD)^2
\]

Results of a Prismatic Lithium-Ion Cell

Geometry & Mesh

Temperature

Current Density

2 Ah Prismatic Cell Discharge Curve
Inputs to Single Cell Thermal Model

- U and Y curves are the inputs to the cell thermal model. U and Y curves are converted from battery performance data.

- A small program has been written to convert the performance data into the U and Y curves needed by Fluent.

\[
U = a_0 + a_1(DOD) + a_2(DOD)^2 + a_3(DOD)^3
\]

\[
Y = a_4 + a_5(DOD) + a_6(DOD)^2
\]
What Performance Data Needed?

• Short answer: **Battery discharge curves.** (aka polarization characteristics)

• Precise answer: Battery cell potential as a function of depth of discharge (DOD) for different discharge rates sampled in the way demonstrated in Gu’s paper Figure 3.

• The required data can be from either testing or electrochemistry model.

Battery discharge curves are battery cell potential as a function of capacity, time, or DOD for different discharge rates.

The two examples use capacity and time. But we need DOD!!
What is DOD?

Definition of depth of discharge (DOD) used:

\[ DOD = \frac{\int_{0}^{t} Jdt}{Q_t} \]

What is \( Q_t \)?

- The theoretical capacity per unit area of the electrodes.
- Achieved when cell potential is lower than certain value discharged at a rate close to zero.
These results are from Newman electrochemistry model in Simplorer.
Discharge Curves in DOD
Sampled Discharge Curves in DOD

Simplorer offers nice sampling tools shown above.
Data Input File Format to the Program

Matrix Size

<table>
<thead>
<tr>
<th>DOD</th>
<th>Main Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000</td>
<td>11.8</td>
</tr>
<tr>
<td>0.0100</td>
<td>0.02750</td>
</tr>
<tr>
<td>0.0840</td>
<td>1.72500</td>
</tr>
<tr>
<td>0.1800</td>
<td>1.73536</td>
</tr>
<tr>
<td>0.2830</td>
<td>1.61484</td>
</tr>
<tr>
<td>0.3920</td>
<td>1.59406</td>
</tr>
<tr>
<td>0.5090</td>
<td>1.54060</td>
</tr>
<tr>
<td>0.6180</td>
<td>1.48542</td>
</tr>
<tr>
<td>0.7150</td>
<td>1.43209</td>
</tr>
<tr>
<td>0.8050</td>
<td>1.25200</td>
</tr>
<tr>
<td>0.8690</td>
<td>0.67567</td>
</tr>
</tbody>
</table>

Current Density

Not Used
Program Output: Polynomial Coefficients for U and Y

Coefficients for U

\[ \text{coeff for U. The matrix has 4x1 elements} \]
\[
\begin{array}{c}
4.187e+000 \\
-1.659e+000 \\
2.661e+000 \\
-2.676e+000
\end{array}
\]

Coefficients for Y

\[ \text{coeff for Y. The matrix has 4x1 elements} \]
\[
\begin{array}{c}
1.570e+002 \\
-8.976e+001 \\
-1.684e+002 \\
1.899e+002
\end{array}
\]

Note that the extraction code allows you to select the order of polynomial. An order of 3 is used for both U and Y.

\[
U = 4.187 - 1.659 \cdot DOD + 2.661 \cdot DOD^2 - 2.676 \cdot DOD^3
\]
\[
Y = 157.0 - 89.76 \cdot DOD - 168.4 \cdot DOD^2 + 189.9 \cdot DOD^3
\]
Curve Fitting Results

U Results

Y Results
Battery electrochemistry can be modeled using VHDL-AMS in Simploter.

Battery cell thermal analysis can be performed using a simplified model in FLUENT.

Model inputs for the cell thermal model can be calculated from battery electrochemistry model.
Thank you!!