Identification of Relevant Parameters for Battery Model using Calibration Under Discharge Condition

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Motivation

• Energy turnaround
  • E-mobility awareness increases
  • Alternative energy sources
    → more and more energy storages are needed

• Weaknesses of energy storages
  • Thermal Runaway
  • Decreasing capacity
  • Small energy density

→ Understand charge and mass transport of batteries before production
→ Simulation of batteries beyond known limits

Quelle: www.sueddeutsche.de


Quelle: www.all-electronics.de
Battery Simulation
Simulation Task – Identification and Calibration

- Newman Model based (LIBERA Project from CADFEM/THI)
  - Lithium-Ion Diffusion
  - Charge transport
  - Electrochemical reaction

- Pseudo 2D-Model:
  **Dimension x:** transport from negative to positive electrode
  **Dimension r:** particles describing porosity of electrodes

Main Output signal: e.g. Voltage vs. charge

- Goal:
  - Identify driving parameters
  - Calibrate signals between simulation and test
 Parametric Workflow for Battery Simulation

- Battery simulation on electrode level
- Input parameters
  - Physical battery model parameters
  - Setup parameters
- Output parameters
  - Voltage vs. time
  - Current vs. time
- Reference Signals
  - 1 C Rate Voltage vs. Charge
  - 2 C Rate Voltage vs. Charge
  - 4 C Rate Voltage vs. Charge

References

- 1 C Rate Voltage vs. Charge
- 2 C Rate Voltage vs. Charge
- 4 C Rate Voltage vs. Charge

Voltage in V vs. Charge in Ahr

Graph showing voltage and charge for different current rates.
Parametric Workflow for Battery Simulation

Parametric System

Battery Parameters → Setup Parameters → Solve → Output Parameters and Signals

Electrode Domain
- Current Collector
- Positive Electrode
- Separator
- Negative Electrode
- Current Collector

Particle Domain

Graph showing output parameters and signals with data points and lines.
• 13 Input Parameter

• Which parameters influence the discharge signal?

→ Sensitivity analysis

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Reference Value</th>
<th>Lower Bound</th>
<th>Upper Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>D_e</td>
<td>electrolyte phase Li-ion diffusion coefficient</td>
<td>m²/s</td>
<td>7.50E-11</td>
<td>3.00E-11</td>
<td>1.20E-10</td>
</tr>
<tr>
<td>Ds_n</td>
<td>diffusion coefficient at the solid phase. negative electrode</td>
<td>m²/s</td>
<td>3.90E-14</td>
<td>1.56E-14</td>
<td>6.24E-14</td>
</tr>
<tr>
<td>Ds_p</td>
<td>diffusion coefficient at the solid phase. positive electrode</td>
<td>m²/s</td>
<td>1.00E-13</td>
<td>4.00E-14</td>
<td>1.60E-13</td>
</tr>
<tr>
<td>ep_n</td>
<td>volume fraction of electrolyte at the negative electrode</td>
<td>-</td>
<td>0.357</td>
<td>0.143</td>
<td>0.571</td>
</tr>
<tr>
<td>ep_p</td>
<td>volume fraction of electrolyte at the positive electrode</td>
<td>-</td>
<td>0.444</td>
<td>0.266</td>
<td>0.622</td>
</tr>
<tr>
<td>epf_n</td>
<td>volume fraction of filler material at the negative electrode</td>
<td>-</td>
<td>0.172</td>
<td>0.103</td>
<td>0.241</td>
</tr>
<tr>
<td>epf_p</td>
<td>volume fraction of filler material at the positive electrode</td>
<td>-</td>
<td>0.259</td>
<td>0.104</td>
<td>0.414</td>
</tr>
<tr>
<td>k_n_ref</td>
<td>electrochemical reaction rate constant of negative electrode</td>
<td>mol/m²/s/(mol/m³)¹.5</td>
<td>2.33E-11</td>
<td>9.32E-12</td>
<td>3.37E-11</td>
</tr>
<tr>
<td>k_p_ref</td>
<td>electrochemical reaction rate constant of positive electrode</td>
<td>mol/m²/s/(mol/m³)¹.5</td>
<td>2.33E-11</td>
<td>9.32E-12</td>
<td>3.73E-11</td>
</tr>
<tr>
<td>Rs_n</td>
<td>particle radius in negative electrode</td>
<td>m</td>
<td>1.25E-05</td>
<td>5.00E-06</td>
<td>2.00E-05</td>
</tr>
<tr>
<td>Rs_p</td>
<td>particle radius in positive electrode</td>
<td>m</td>
<td>8.00E-06</td>
<td>3.20E-06</td>
<td>1.28E-05</td>
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<tr>
<td>sigma_n</td>
<td>electrical conductivity of negative electrode</td>
<td>S/m</td>
<td>100</td>
<td>90</td>
<td>110</td>
</tr>
<tr>
<td>sigma_p</td>
<td>electrical conductivity of positive electrode</td>
<td>S/m</td>
<td>3.80</td>
<td>3.42</td>
<td>4.18</td>
</tr>
</tbody>
</table>
Simultaneous Simulation Workflow for all 3 C-Rates

- Sensitivity analysis with 200 designs
Characterization of Calculated Signals

channel 0 of signal C4_SIM_Charge_Voltage
• Non-physical convergence problems → unconverged solution
• New check output parameter: if converged then 0 otherwise -1
• Unconverged Signals are neglected
• Limit of 2.75 V is not reached
• Additional check output parameter: if limit reached then 0 otherwise -1
• Limit of 2.75 V is not reached
• Signals are neglected
Characterization of Calculated Signals

- All remaining signals
  - converged
  - reached 2.75 V
  - Both check output parameters = 0

BUT

Signal lengths differ!
• All remaining signals
  • converged
  • reached 2.75 V

Extrapolation of calculated signal to compensate difference between reference and simulation result?
Characterization of Calculated Signals

• All remaining signals
  • converged
  • reached 2.75 V

Extrapolation is NO option!
There is a solution for this problem!
Characterization of Calculated Signals

- Transpose signal
- All signals have same length
- No extrapolation – raw data from simulation
- Calibration possible
Calibration – Minimize Difference between Reference and Simulation

- Root Mean Squared Error RMSE (normalized) \( \triangleq \) Difference

\[
RMSE = \sigma \varepsilon = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i^* - y_i)^2}
\]

- \( n \): Number of data points
- \( y^* \): Reference value (measurement)
- \( y \): Calculated value (battery simulation)

\( \rightarrow \) Optimization task: Minimizing the difference for all necessary data points
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter 1 C rate = -1 are deselected
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter 2 C rate = -1 are deselected
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter 4 C rate = -1 are deselected
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter for all C rates = -1 are deselected
Identification of non-valid Designs

• Parallel Coordinates Plot
  • Select designs with low difference values → new lower and upper bounds
2nd Sensitivity with Reduced Parameter Bounds

- 1st sensitivity with 200 designs
  - Statistics
    - Unconverged solutions: 34
    - Limit of 2.75 V not reached: additional 128 designs
    - Non-valid designs: 162
    - Valid designs: 38

- 2nd sensitivity with 200 designs
  - Reduction of parameter bounds based on designs with low difference values
    → Identify parameters with high influence on the signal
  - Statistics
    - Unconverged solutions: 0
    - Limit of 2.75 V not reached: additional 69 designs
    - Non-valid designs: 69
    - Valid designs: 131
Influence of Input Parameters on Signal

- Linear correlation matrix
- Resolution of signal with 500 sampling points
Influence of Input Parameters on Signal

- COP Matrix
  - 11 important parameters
  - 2 unimportant parameters (D_e and sigma_p)
Calibration – Minimize Difference between Reference and Simulation

• Dividing signals in 2 parts
  • Differenced for part 1 and part 2 for all C rates

• Restrictions
  • All check output parameters \( \geq 0 \)

• Weighting factors: \( W_i \)
• Normalizing factors: \( N_i \) (max y-value minus min y-value)

• Objective function
  • \( \min (W_1 \cdot C_1 \text{ Difference\_Part 1}/N_1 + W_2 \cdot C_1 \text{ Difference\_Part 2}/N_2 \ldots) \)
• Adaptive Response Surface Optimization
• Transposed 1 C Rate
Optimization Results

1 C Rate

2 C Rate

4 C Rate
• Parametric simultaneous simulation of battery discharge behavior for different C rates

• Signal lengths differ → transposing signals

• Sensitivity reveals parameters influencing the signal characteristic

• Minimizing the difference between reference and simulation by optimization
• Determination of battery parameters
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