Using Battery Design Studio for Battery Simulation and New Features
xEV simulations require estimates of battery electrical and thermal behavior.

BDS cell design process.
- Physical cell description
- Fitting model parameters

Model Improvements
- NTGP
- RCRTable
- DISTNP

Conclusions
The drive cycle represents a typical work-home commute which starts in a suburban area, characterized by UDDS, then continues on a highway, simulated by HWFET, and finally arrives to downtown urban area, UDDS.


Challenge: Model electrothermal behavior of battery.
Selected Simulation Models in Battery Design Studio

**Cell Design**
- **DISTNP**
  - Solves transport, kinetics, equations

**HEV/PHEV Module/Pack**
- **RCR**
  - Quick response for frequent charge/discharge like HEV/PHEV energy storage

**EV Module/Pack**
- **NTG**
  - Simple, easy to create model, and best for simple discharging thermal analysis

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2. Battery Design LLC, “BDS Documentation”

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\[ J = Y \left( V_p - V_n - U \right) \]
\[ U = a_0 + a_1(DOD) + a_2(DOD)^2 + a_3(DOD)^3 \]
\[ Y = a_4 + a_5(DOD) + a_6(DOD)^2 \]

Physical Cell Description
• Coin, cylindrical pouch, prismatic
• Gives size, weight, equilibrium voltage, capacity, bill of materials, etc.

Fit Model Parameters
• circuit, physics
• Allows simulation of performance

Use and/or Distribute

Text Battery Model (tbm)
TBM files bridge the design process for batteries

Battery Design Studio

Materials Developers
- Button cell
- Active materials
- Additives
- Electrolytes
- Separator

Cell Designers
- Model selection
- Electrodes, incl. tabbing
- Separator
- Spiral cylindrical, prismatic, stack

Module/Pack Developers
- Series/Parallel cells
- CFD with heat transfer

End Users
- System simulation

STAR-CCM+

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Simple Cell – useful for coin cell simulation

Materials developers typically use coin cells

Stainless steel lid

Spring

Spacer

Lithium foil. 1.5875 cm dia
Separator, 1.9 cm dia, 100 um
Cathode, 1.27 cm dia

Stainless steel case

1 M LiPF6/EC:DEC (1:1 volume)

Key properties
- Density
- Voltage
- Surface area
- Diffusion coeff.
Fitting solid-phase diffusion coefficient of lithium nickel cobalt aluminum oxide

Pulse experiments done in coin cells can be used to fit solid-phase diffusion coefficients of active materials.

Y. Li (FMC), Star Global Conference 2012 Amsterdam
Electrolyte Models
- AEM computed property sets from K. Gering

EC3_EMC7_LiFSI
EC3_EMC7_LiPF6
EC31_PC10_DMC59_LiPF6
EC23_PC21_DMC56_05LiDFOB_05LiPF6
EC32_DEC23_DMC24_EP22_LiPF6
EC38_DMC31_EMCEMC31_05LiPF6_05LiFSI
EC31_EMCEMC46_DEC23_LiFSI
EC31_EMCEMC46_DEC23_LiPF6
EC39_EMCEMC30_DMC30_LiPF6
EC15_EMCEMC64_GBL21_LiFSI
PC58_DME42_LiTFSI
PC58_DME42_LiCF3SO3

Electrolyte properties available in next release of BDS.
Comparison of Gering’s computed properties with literature values

Experimental values for electrolyte properties can be directly entered in tabular form.
Physical Cell Description: Stacked Plate Cells

Parameter | Value  
---|---
Height (h), mm | 149.000
Width (w), mm | 86.000
Tab offset (Otab) | 3.000
Tab width (wtab), mm | 35.000
Tab height (htab), mm | 20.000
Coat. offset (Ocoat), mm | 0.000

End Electrodes: Both Negative | Left end | 37
Both Positive | Right End
Pos(right)/Neg |
Physical Cell Description: Spirally-Wound Cells - Tabbed electrode

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>S1, mm</th>
<th>S2, mm</th>
<th>S3, mm</th>
<th>S4, mm</th>
<th>S5, mm</th>
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</tbody>
</table>
Physical Cell Description: Spirally-Wound Cells - Multi-tabbed electrode
Physical Cell Description: Spirally-Wound Cells - Edge Collector with clamp

Available in next release of BDS.
Polynomial fits introduce significant error.
Bezier curves conform to parameter values exactly. Parameter input is simplified since only values need to be provided.
Comparison of data and fitted (NTG model) voltage behavior for cell with 100 micron thick cathode coating.

Comparison of data and fitted (NTG model) voltage behavior for cell with 100 micron thick cathode coating.

NTGP model improves fit to data when discharge or charge capacity depends on rate.
RCR Table – an enhanced RCR model

RCR Model

\[ C = \frac{\tau}{R_p} \]

Enhancements provided by RCRTable

- Enter model parameters at specific SOC values directly, no need to fit to polynomials
- Use linear interpolation for temperature dependence
- Polarization resistance can depend on current (rate or Tafel effect)
- Warburg impedance
  \[ \Rightarrow \text{Capability to fine tune fits to data} \]

RCR model is useful for simulating performance of HEV batteries

- Parameters are a function of SOC represented by polynomials
- Parameters depend on temperatures via Arrhenius relation

Cell resistance decreases with increasing current

\[ R_{p,1} = R_{p,0} \left( \frac{1}{|i|} + \exp\left( - \frac{|i|}{i_0} \right) \right) \]

- \( R_{p,1} = \) Polarisation resistance
- \( R_{p,0} = \) Polarisation resistance at zero current
- \( i_1, i_0 = \) Adjustable parameters

<table>
<thead>
<tr>
<th>Current, A</th>
<th>Resistance, mOhms</th>
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<tr>
<td>50</td>
<td>2.122</td>
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<tr>
<td>100</td>
<td>1.473</td>
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RCRTable Model: Warburg Effect

Cell resistance increases with time.

\[ R_p = \frac{R_{p,1}}{1 + R_{W}} \]

\[ R_W = A_d \sqrt{\frac{t}{e^{B_d} - e^{V_{oc}}}} \]

\( R_{p,1} \) = Polarisation resistance
\( R_W \) = Warburg impedance
\( A_d \) & \( B_d \) are coefficients

\( V_{oc} \) is related to the OCV curve

Volts vs. Time

Time (min)
DISTNP Model: SEI Growth

• Sei growth by solvent reduction is one dominant aging mechanism in Li-ion batteries:
  • increase in cell resistance
  • irreversible consumption of available Lithium
• deterioration in:
  • capacity
  • rate capability
• experimental investigations have shown a sqrt(t) dependency
• a new SEI growth feature was implemented in BDS using a diffusion based transport model after Ploehn et al. (J. Echem. Soc. 151(3) A456 (2004))
• feature available for Li_Pouch_dist1D in release 8.02 but will be available for other Dist models (in STAR CCM+ as well)


New SEI growth parameters in the particle

<table>
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<tr>
<th>Parameters</th>
<th>I</th>
<th>X</th>
<th>+</th>
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<td>Buffer Volume</td>
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<td>PreExp Factor, mA/cm²</td>
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<td>Cathodic Transfer Coefficient</td>
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<td>SEI</td>
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<td>O</td>
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<tr>
<td>PooIh</td>
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<td>SEI Initial Thickness (A)</td>
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<td>Solvent Diffusion Anhynous Coefficient (k/min)</td>
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<td>Solvent Diffusion Activation Energy (1/kmol)</td>
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<td>Solvent Diffusion Concentration (mol/m³)</td>
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<td>SEI Product Concentration (mol/m³)</td>
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</table>

Graph showing SEI growth parameters over time at 15°C, 30°C, and 60°C.
Notes on the required input data

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<td>Anodic Transfer Coefficient</td>
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<td>Cathodic Transfer Coefficient</td>
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<td>Double-layer Capacitance, F/m²</td>
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<td>SEI</td>
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<td>SEI Pre-Exp. Factor, ohm-cm²</td>
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<td>None</td>
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<td>Solvent Diffusion Arrhenius Coefficient (m²/s)</td>
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<td>SEI Product Concentration (mol/m³)</td>
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</table>

Model on or off
Initial SEI thickness specified by user
Values taken from Ploehn paper

Running with the ‘long report’ or ‘solid-phase profiles’ option produces a very large *.pr2 file (circa 2GB in this case)
Run time is considerably effected by frequency of report in .prg file

Changed to 1 day, which expedites the aging run time and file size
After simulation is run, ‘aged’ tbm file can be found in the BDS Results directory.

Thickness is increased compare to original and this tbm file could then be used in STAR-CCM+ BSM to represent an aged cell.

Run a capacity test on both new and aged tbm files to see effect.
Conclusions

- BDS provides models to simulate electrothermal behavior of batteries useful for design of automotive batteries.
- BDS provides pathway for materials suppliers to provide design parameters to cell developers, and cell developers to provide cell models to pack developers.
- BDS enables physical cell descriptions that accurately represent actual designs.

New features of BDS
- BDS allows modeling of tabbing arrangements for spirally-wound cells.
- BDS provides electrolyte property systems to aid in physics-based simulation of lithium-ion cells.
- BDS provides accurate representation of parameter dependence for NTG and RCR models on state of charge.
- BDS allows simulation of impedance growth due to SEI growth.