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CONVERGE CFD for Battery Simulations

- CONVERGE CFD software is well-suited for battery simulations of 3D coupled flow, heat transfer, and chemistry in complex geometries, with autonomous mesh generation to reduce total time-to-solution.

- CONVERGE contains the SAGE detailed chemical kinetics solver, parallelized efficiently for fast run-times and adopted to model battery vent gas combustion and thermal runaway chemistry inside the solid.

- Adaptive mesh refinement (AMR) automatically resolves the flow, diffusion of vent gas, flame front and thermal runaway front propagation at low computational expense.

- Wide variety of other physics-based 3D modeling capabilities that have been utilized for battery simulations.
Thermal Runaway Propagation and Vent Gas Simulations

Capturing Battery Thermal Runaway and Venting Phenomena using Detailed 3D CFD Solutions

Kislaya Srivastava et.al,
2022 NASA Aerospace Battery Workshop
Phase-Change Materials: An Overview

- Heat storage device: Absorbs heat during melting, releases heat during solidification
  - Temperature regulators
- Passive cooling approach: Lightweight, compact, efficient, consistent, sustainable
- Versatile: Variety of PCMs with broad spectrum of transition temperatures
  - Selection based on optimal battery operating temperature
- Drawbacks: Low conductivity, possible leakages, possible structural failures at high temperatures
- Conductivity/heat transfer can be enhanced using fins
PCMs with CFD: Solidification and Melting Model

- Solid-liquid phase change modeled using the enthalpy-porosity method
- Porosity of PCM:
  - 1: Solid, $T < T_{\text{solidus}}$
  - 0: Liquid, $T > T_{\text{liquidus}}$
  - Between 0 and 1: Mushy zone with liquid volume fraction, $T_{\text{solidus}} < T < T_{\text{liquidus}}$
- Liquid flow modeled as laminar and incompressible Newtonian fluid
- Boussinesq approximation to model buoyancy effect
- Transient 3D conjugate heat transfer simulations of PCM battery cooling investigated

PCM: Paraffin wax (melting range: 314-317K)
Battery Equivalent Circuit Model

- Lumped-parameter model for electrothermal response
  - Simplistic and computationally inexpensive, empirical
  - Lin. et. al., “A lumped-parameter electro-thermal model for cylindrical batteries”
  - Represent battery as an electrical network and calculate heat source based on current (charging or discharging)
  - Inputs: battery capacity, initial SOC, current profile, 1D/2D data tables

Terminal voltage:

\[ V_T = V_{OCV} - IR_S - \sum_{i=1}^{n} V_{RC,i} \]

\[ \frac{dV_{RC,i}}{dt} = -\frac{1}{R_i C_i} V_{RC,i} + \frac{1}{C_i} I \]

\[ \frac{dSOC}{dt} = -\frac{1}{C_{bat}} I \]

\[ Q = I(V_{OCV} - V_T) \]
PCM Simulations : Results (1/2)

BEC for battery heat release under a discharge cycle
PCM : Paraffin wax (melting range : 314-317K)
PCM Simulations : Results (2/2)

BEC for battery heat release under a low C-rate charge cycle
PCM : Paraffin wax (melting range : 314-317K)

Temperatures within the PCM material

Temperature regulation (warming) during cooldown : Latent heat released during solidification
## PCM Material Selection

<table>
<thead>
<tr>
<th>Material</th>
<th>Temp_liquidus (K)</th>
<th>Temp_solidus (K)</th>
<th>Specific Heat Capacity (K/Kg.K)</th>
<th>Latent heat capacity (J/kg)</th>
<th>Density (Kg/m3)</th>
<th>Conductivity (W/mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paraffin</td>
<td>317.15</td>
<td>314.15</td>
<td>2000</td>
<td>255000</td>
<td>880</td>
<td>0.13</td>
</tr>
<tr>
<td>RT50</td>
<td>324.15</td>
<td>318.15</td>
<td>2950</td>
<td>168000</td>
<td>880</td>
<td>0.19</td>
</tr>
<tr>
<td>N-Eicosane</td>
<td>310.50</td>
<td>306.50</td>
<td>1926</td>
<td>248000</td>
<td>910</td>
<td>0.423</td>
</tr>
<tr>
<td>Lauric acid</td>
<td>321.35</td>
<td>316.65</td>
<td>2180</td>
<td>187210</td>
<td>940</td>
<td>0.16</td>
</tr>
</tbody>
</table>

The graph shows the mean temperature (K) over time (seconds) for each material.
Addressing PCM Drawbacks: Low Conductivity

- Composites
- Addition of fins

<table>
<thead>
<tr>
<th></th>
<th>Conductivity (W/m.K)</th>
<th>Specific heat capacity (J/Kg.K)</th>
<th>Latent heat capacity (J/kg)</th>
<th>Temp liquidus (K)</th>
<th>Temp solidus (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT44HC</td>
<td>0.21</td>
<td>2250</td>
<td>270000</td>
<td>317.15</td>
<td>314.15</td>
</tr>
<tr>
<td>CPCM</td>
<td>11.00</td>
<td>2500</td>
<td>107800</td>
<td>318.15</td>
<td>314.15</td>
</tr>
</tbody>
</table>
Fluid Dynamics Within PCMs
Fluid Dynamics Within PCMs: Natural Convection (2/2)
Fin Design Improvements : Helical Fin
Fin Design Improvements: Double Helical Fin (1/2)
Fin Design Improvements: Double Helical Fin (2/2)
Incorporating 3D Effects: Short-Circuit Model

• Time or Temperature (ISC device) controlled short-circuit event, independent shape/size (for heat release)
• Resistance $R_{SC}$: User input

ISC@240s, TR onset @250s

![3D Model and Temperature Distribution](image-url)

- **TEMPERATURE**
  - 1200
  - 1100
  - 1050
  - 1000
  - 950
  - 900
  - 850
  - 800
  - 750
  - 700
  - 650
  - 600
  - 550
  - 500
  - 450
  - 400
  - 350

- **Graph**
  - Y-axis: $S_D$
  - X-axis: Time (seconds)
  - Lines:
    - noShort
    - wShort_RISC0.1
    - wShort_RISC0.05
    - wShort_RISC0.025

![Graph](image-url)
PCM/Fin Assembly Response to Short-Circuit Location

*Thermal runaway model inactive*
Non-Uniform Battery Heating
$\nabla (\sigma \nabla \phi_1) = S (\phi_1, \phi_2)$

$\nabla (\sigma \nabla \phi_2) = -S (\phi_1, \phi_2)$

$E_1 = -\nabla \phi_1$

$E_2 = -\nabla \phi_2$

$Q = \sigma E_1^2 + \sigma E_2^2 + q_{elec}$

$\phi_1: 4.05V$

$\phi_2: \text{Zero NE}$

$\phi_1: \text{Zero NE}$

$\phi_2: 0.0V$
Coupled Electric Potential Solver: A 3D Analysis (2/2)
Thermal Runaway Mitigation with PCMs

- Thermal runaway reaction model utilized for a predictive analysis
- Are TR simulation results reliable? : Reproducibility and repeatability
Thermal Runaway Propagation Analysis: Chemistry

- Thermal runaway reaction kinetics
  - Hatchard-Kim mechanism: 4 Reactions, LCO battery chemistry

\[
R_{\text{sei}}(T, c_{\text{sei}}) = A_{\text{sei}} \exp \left[ - \frac{E_{a,\text{sei}}}{RT} \right] c_{\text{sei}}^{m_{\text{sei}}}
\]

Anode and electrolyte (ne)
\[
R_{\text{ne}}(T, c_{\text{e}}, c_{\text{neg}}, t_{\text{sei}}) = A_{\text{ne}} \exp \left[ - \frac{t_{\text{sei}}}{t_{\text{sei},\text{ref}}} \right] c_{\text{neg}}^{m_{\text{ne,n}}} \exp \left[ - \frac{E_{a,\text{ne}}}{RT} \right]
\]

Cathode and electrolyte (pe)
\[
R_{\text{pe}}(T, \alpha, c_{\text{e}}) = A_{\text{pe}} \alpha^{m_{\text{pe,p1}}(1 - \alpha)^{m_{\text{pe,p2}}}} \exp \left[ - \frac{E_{a,\text{pe}}}{RT} \right]
\]

Electrolyte decomposition (e)
\[
R_{e}(T, c_{\text{e}}) = A_{e} \exp \left[ - \frac{E_{a,e}}{RT} \right] c_{\text{e}}^{m_{e}}
\]

- Calibrated reaction mechanisms required to reproduce experimental behavior
  - Reliant on experimental DSC data

- A comprehensive species-based reaction mechanism for thermal runaway chemistry?
Thermal Runaway Propagation Analysis: Statistics

Raw data from the ARC experiment

<table>
<thead>
<tr>
<th>Batt</th>
<th>Exotherm onset Temp° T_{onset} (°C)</th>
<th>Thermal runaway onset Temp° T_{onset} (°C)</th>
<th>Max Temp° T_{max} (°C)</th>
<th>TR delay time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batt 1</td>
<td>118.17</td>
<td>211.38</td>
<td>385.38</td>
<td>204.33</td>
</tr>
<tr>
<td>Batt 2</td>
<td>97.73</td>
<td>210.06</td>
<td>716.45</td>
<td>720.5</td>
</tr>
<tr>
<td>Batt 3</td>
<td>67.58</td>
<td>199.98</td>
<td>345.13</td>
<td>1300.96</td>
</tr>
<tr>
<td>Batt 4</td>
<td>123.83</td>
<td>220.94</td>
<td>456.48</td>
<td>121.52</td>
</tr>
<tr>
<td>Batt 5</td>
<td>77.99</td>
<td>201.14</td>
<td>384.15</td>
<td>897.45</td>
</tr>
<tr>
<td>Batt 6</td>
<td>77.44</td>
<td>195.96</td>
<td>392.72</td>
<td>602.80</td>
</tr>
<tr>
<td>Batt 7</td>
<td>76.89</td>
<td>226.62</td>
<td>390.33</td>
<td>1584.35</td>
</tr>
<tr>
<td>Batt 8</td>
<td>77.54</td>
<td>200.65</td>
<td>726.68</td>
<td>911.74</td>
</tr>
<tr>
<td>Batt 9</td>
<td>77.47</td>
<td>204.19</td>
<td>414.42</td>
<td>1044.03</td>
</tr>
</tbody>
</table>

Statistical analysis of frequency factor and global activation energy of all 16650 Samsung LCO cells.

\[
\frac{dc}{dt} = -A e^{-\frac{E}{RT}}
\]

\[
\frac{dT}{dt} = H A e^{-\frac{E}{RT}}
\]

Zhang et. al. (2022)
PCMs as Fire Retardants

- Possible use of PCMs as flame retardants
- CONVERGE has established surface chemistry capabilities that can be utilized
- But what ignites the gases?

Spark ignited vent gas combustion inside a battery pack
Self ignition of vent gases after exit
Vent gas ignition due to hot ejecta
Thermal Interactions Between Solid Ejecta and PCM

- Lagrangian solid particle wall film modeling approach for deposition of solid ejecta during thermal runaway and associated heat transfer to walls
THANK YOU!
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