How to effectively use AutoLion-3D™ if user is interested in simulating cell voltage change with time

**Introduction**

Many of AutoLion-3D™ users sometimes want to use this software to simulate performance of a cell and compare results with experimental data. Three-dimensional cell modeling, as in AutoLion-3D™, is computationally intensive especially if a user is interested in simulating standard performance such as cell voltage change with time when subjected to a constant current charge-discharge current. We, however, understand that users may want to use AutoLion-3D™ for such purposes from time-to-time to gain confidence or to tune the model parameters to obtain a better match with data. There is a much more computationally effective way of using AutoLion-3D™ to simulate typical performance behavior i.e. using “pack model” feature in AutoLion-3D™. This case study is designed to show how users can utilize “pack model” feature in AutoLion-3D™ to quickly simulate performance characteristics.

**Problem Statement**

Electrochemical performance can be simulated in AutoLion-3D™ using either cell model or through 1 cell pack model. The differences between these two models are explained in details in the user manual. Simply put, 1) the cell model is a full 3D model and all the variables are solved over the three-layers of 3D meshes and 2) Pack model, on the other hand, solves the thermal field in 3D but the electrochemical parts in 1D. So pack model runs faster than cell model assuming similar grids are used.

Here we simulate the performance of an 18650 LCO-Graphite cell using 3D cell model as well as through setting up a pack with only one cell. The results are then compared to each other. It is demonstrated that for cell performance, pack model could be a good alternative of 3D cell model without much loss in accuracy but with huge benefits in terms of time and cost.

**Setup**

- A 2.3Ah LCO-Graphite 18650 cell is set up in AutoLion 3D™ in both cell model and pack model.
- The mesh (shown in Figure 1) for cell model is automatically generated using AutoLion 3D™ GUI mesh script and ICEMCFD (Refer to the user manual on automated mesh generation of single cell model).
- A simple trick is used to quickly generate mesh for one-cell pack. The mesh used for pack model is converted from the cell model mesh by merging all the zones except the zone of the cell case. In this way, the meshes used in both models are identical to each other. In practice, pack mesh can also be generated by users.
- The cell is air cooled and the ambient air temperature is 25°C. Convective heat transfer boundary is used with a coefficient of 20 W/(m²*K).
- The cell has an initial SOC of 1.0. A constant 1C rate discharge is then performed.
- Ansys Fluent V14.5 is used as the CFD solver.

**Results**

Table 1 shows the simulation setup and total computation resources used for pack and cell model. The test is carried out on an Intel X5650 2.6 GHz workstation with 23 CPU cores. As can be seen from Table 1, pack model runs significantly faster than cell model with serial. With parallel computing with pack model, it can run even faster, which saves huge amount of time in cell design process.
Table 1 Cell and Pack model comparison

<table>
<thead>
<tr>
<th>Model</th>
<th>Running Model</th>
<th>Total CPU Core used</th>
<th>Total Computation Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell</td>
<td>Serial</td>
<td>1</td>
<td>3 hours</td>
</tr>
<tr>
<td>Pack</td>
<td>Serial</td>
<td>1</td>
<td>1.5 hours</td>
</tr>
<tr>
<td>Pack</td>
<td>Parallel</td>
<td>4</td>
<td>0.5 hour</td>
</tr>
</tbody>
</table>

Figure 2 shows the voltage curves from 3D cell model and 1 cell pack model. The voltage curve predicted by both models match each other extremely well. Also the predicted capacity of the cell is very accurate for both models. So basically the pack model generates pretty much the same voltage curve as cell model but with only a fraction of the computation time in this case.

Figure 3 shows the maximum temperature comparison between the cell model and pack model. Again these two models generate pretty similar results. There is some small discrepancy after 500s but largely these two curves agree with each well and the largest difference is about 1°C. The slight difference in temperature is caused by slight differences in the specified thermal properties for the two models.

Based on these results, pack model can be used as a good alternative of cell model in terms of cell performance simulation. It runs much faster (at least 2 or 3 times faster) than cell model and can provide voltages, capacities and temperatures outputs as accurate as cell model.

**Benefits**

- Simulation performed in approximately half an hour for pack model (one cell) and three hours for cell model with the specified computing resources.
- AutoLion-3DM™ can be utilized with different computational efficiencies depending on the objective of the problem at hand.
- Pack model provides a more effective way of evaluating any cell performances than cell model if no 3D effect needs to be studied.
- 3D cell model although computationally intensive offers three-dimensional distribution of current and other species. Especially at high current it is of great interest to many users to understand three-dimensional distribution and active material utilization. For such an objective, 3D cell model is more appropriate than using pack model with one cell.