# Numerical Simulation to Accelerate (H)EV Battery Development

The lithium-ion battery is a preferred candidate as a power source for hybrid electric vehicle (HEV) and electric vehicle (EV) due to its outstanding characteristics such as high energy density, high voltage, low self-discharge rate, and good stability. However, the HEV and EV market requires much larger lithium-ion batteries than those available in the market for consumer electronics. The possibility of significant temperature increases in large batteries during high power extraction, or even the risk of thermal runaway, is currently one of the major concerns confronting development of lithium batteries for electric vehicles. So, electric engineers need an accurate and yet simple to use thermal model that couples with their battery electric circuit model. **Xiao Hu, Lead Engineer, ANSYS Inc., Canonsburg, USA**

**A properly designed thermal** management system is crucial to prevent overheating and uneven heating across a large battery pack, which can lead to degradation, mismatch in cell capacity and potentially thermal runaway. Design of the thermal management system therefore requires knowledge about the cooling system as well as the amount of heat that will be generated by cells within the battery pack.

## How simulation can help

Simulation can help on two levels, cell level and system level. Cell level refers to single battery cell, and system level could be either a battery module or a complete battery pack.

At a battery cell level, the focus is on detailed heat generation and temperature distribution within a battery cell. This type of study is pursued mainly by battery manufacturers and battery researchers. Experimental data reveals that the rate of heat generation varies substantially over time throughout the course of charging and discharging. Heat can be generated from internal losses of Joule heating and local electrode over-potentials, the entropy of the cell reaction, heat of mixing, and side reactions. If only the most important effects of Joule heating and local electrode over-potentials are considered, heat generation can be expressed by open

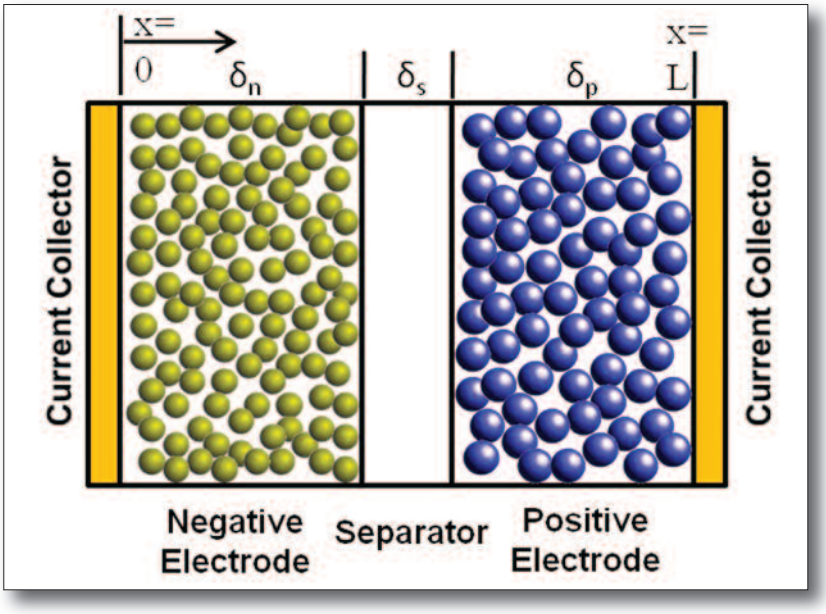


Figure 1: Schematic of a lithium-ion cell

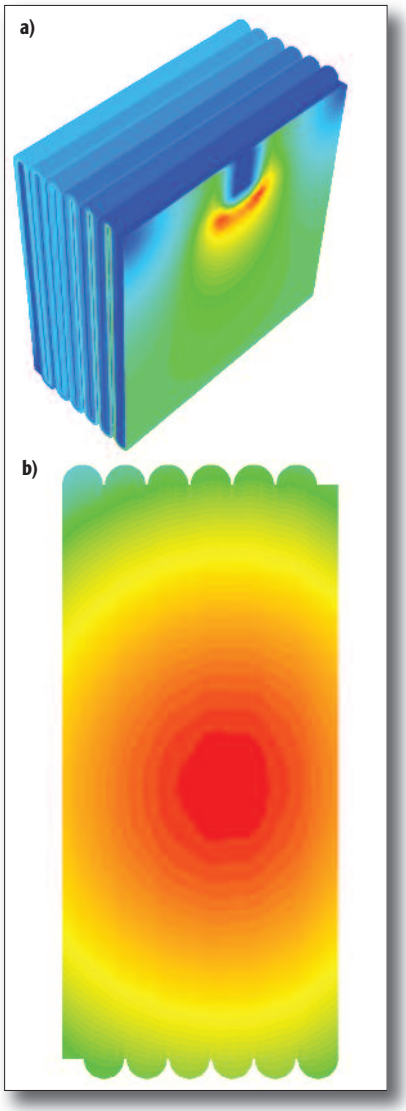


Figure 2: Typical results from models a) pack and b) detail generated in ANSYS® FLUENT®

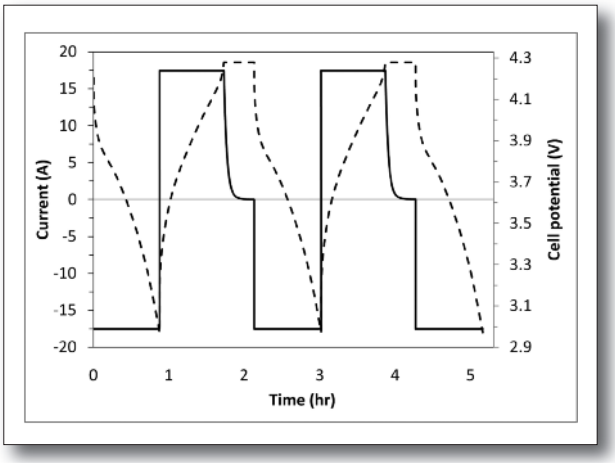


**Figure 3: Charge and discharge cycle results from John Newman's electrochemistry model**

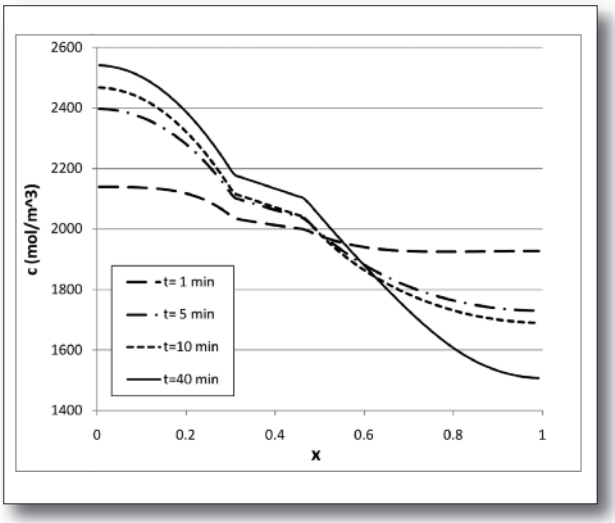


**Figure 4: Concentration profiles during discharge**

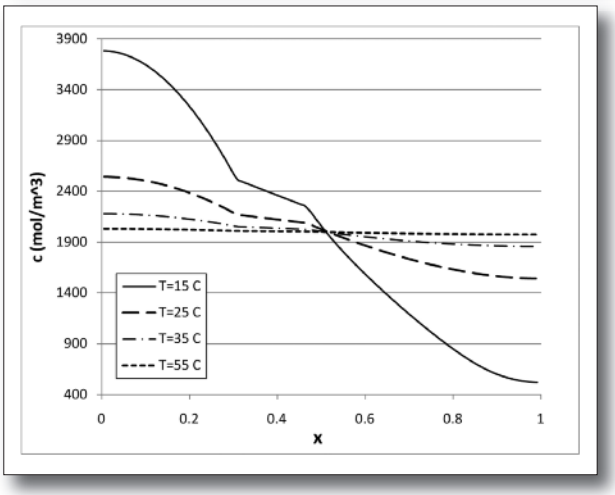


**Figure 5: Concentration profiles under different temperatures**

circuit potential and potential difference between the positive and negative electrodes. Figure 1 shows the schematic of a lithium-ion cell.

Models based on this area can be used to predict the potential and current density distribution on the electrodes of a lithium-ion battery as a function of discharge time. Then, based on the results of the modeling of potential and current density distributions, the temperature distributions of the lithium-ion battery are calculated. The results can then be used to examine the effect of the configuration of the electrodes, such as the aspect ratio of the electrodes and the placing of current collecting tabs as well as the discharge rates on the thermal behaviour of the battery. Figures 2a and 2b show typical results from such models generated in ANSYS® FLUENT®. The temperature distributions from the modeling were shown to be in good agreement with those from the experimental measurement.

While this type of model is simple to use and gives detailed information about temperature and current density distribution, it needs experimental testing data as input. As a result, this type of model cannot predict the impact of design changes on the battery thermal performance without re-conducting the testing. Physics based electrochemistry models, on the other hand, can be used to investigate the impact of battery design parameters on battery performance, which includes the geometry parameters, properties, and most importantly temperature. Physics based models can also provide inputs that would otherwise need experimental testing to obtain.

The most famous physics based model was originally proposed by professor John Newman from UC Berkeley. Such a model has been implemented in Simplorer®. Figure 3 shows charge and discharge cycle results from John Newman's electrochemistry model. Figure 4 shows the concentration profiles during discharge. One optimisation problem that is immediately apparent when examining Figure 4 is the determination of the initial concentration of electrolyte in the cell. The concentration used in Figure 4 is presumably determined due to the conductivity maximum that occurs at approximately this concentration. However, Figure 4 shows that the bulk of the composite cathode is at a significantly lower concentration, where the conductivity is also much lower as a result. This leads to severe transport limitations in the depth of the electrode, suggesting that a higher initial concentration leads to a somewhat lower conductivity in the separator, but a much larger conductivity in the composite cathode, where this is of prime importance. Figure 5 shows the concentration profiles under different temperatures. The information contained in such data tells battery designers when the limiting current occurs, and thus can help specify the temperature range that the cooling system has to maintain to avoid hitting the limiting current.

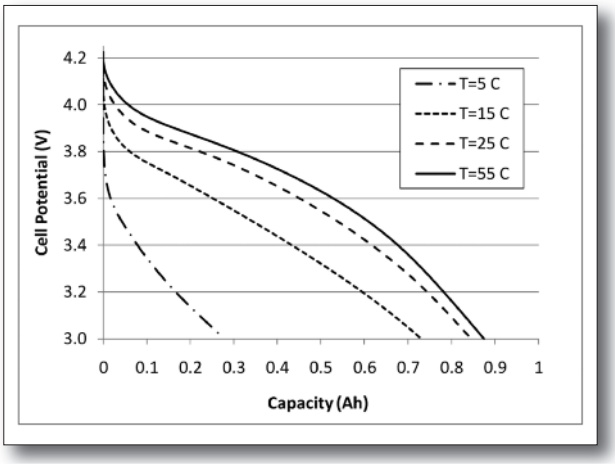


Figure 6: **Cell voltage vs capacity at various temperatures**

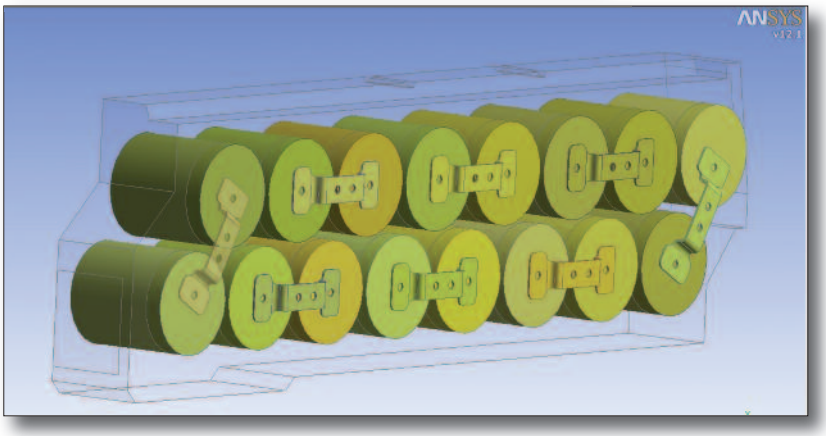


Figure 7: **Simple CFD example**

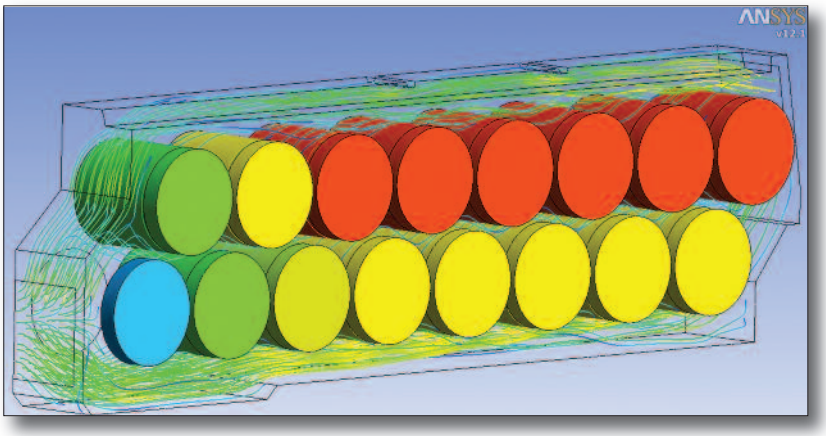


Figure 8: **Complex CFD example**

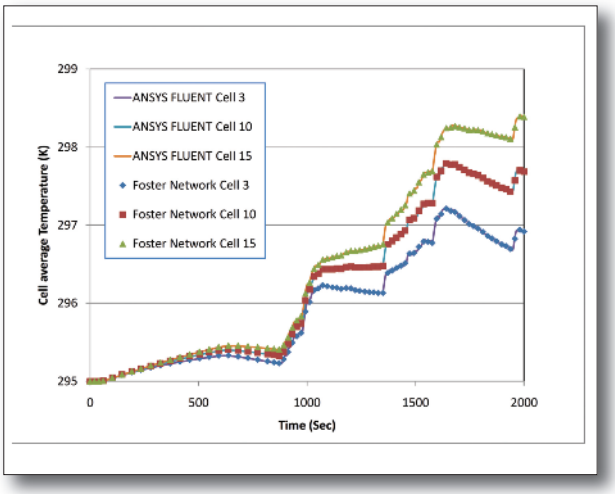


Figure 9: **Comparison between Foster network model and full CFD**

Another implication of Figure 5 is that battery run-time is a strong function of time, and battery life is longer with higher operating temperature. This is also confirmed in Figure 6 from the physics based electrochemistry model. Of course higher temperatures bring safety concerns, and thus this becomes another optimisation problem in battery design.

System level design engineers working at a module or pack level have a different set of requirements. Typically, these engineers cannot afford to simulate as many details as engineers working at the cell level can, and they also have a different set of simulation goals. For instance, Computational Fluid Dynamics (CFD) engineers working in battery thermal management are interested in maintaining the desired temperature range, reducing pressure drop, and maintaining temperature uniformity. And for them, detailed heat generation mechanisms and battery cell structure are not of primary interest. CFD has been widely used for predicting flow and heat transfer, and thus battery thermal management CFD simulation is just another application.

ANSYS has been working to make the process easier for the user. Rather than having to use different tools for geometry, meshing, post-processing, and optimisation, which are all integrated components of a CFD analysis, ANSYS Workbench™ creates all the aspects of the simulation under one umbrella. Geometries built within workbench tools or imported from other CAD packages are all parameterised.

An update of results due to a change of geometric parameters can be achieved in just one click. Data transfer between different simulation tools are handled seamlessly. With the help of ANSYS Workbench, a complete battery thermal CFD analysis, including optimization, can be done entirely within this environment. Figures 7 and 8 show such a CFD example performed by a major automotive OEM.

While CFD can give detailed thermal information about a battery thermal management system, it is time consuming to perform many transient simulations under different drive cycles. Model order reduction techniques exist to extract a model from CFD results, and the extract model, called Foster network model, gives the same solution as that from the full CFD model. However it runs much faster compared with CFD.

For the model shown in Figures 7 and 8, it takes a couple of hours to simulate one drive cycle under one single CPU. But for the extracted Foster network model, the simulation time is reduced to approximately 20 seconds, a time

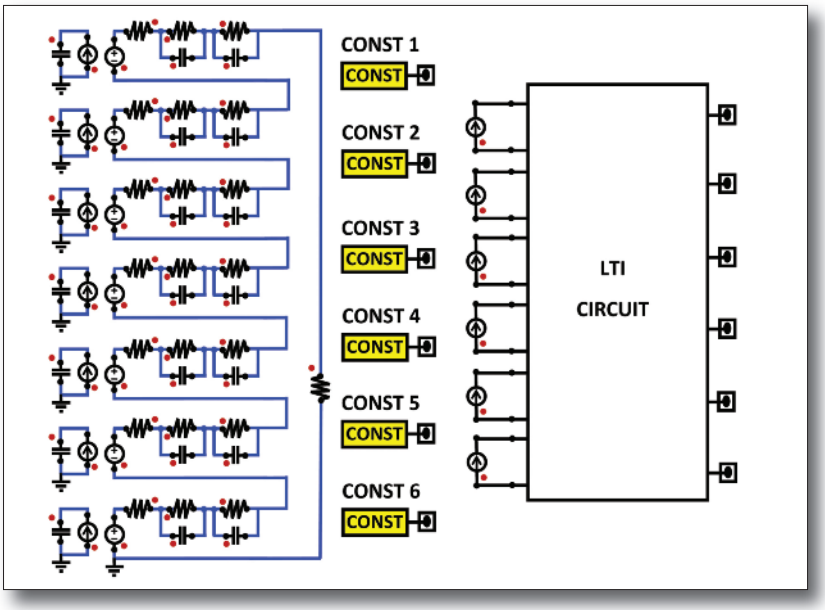


**Figure 10:** Complete dynamic battery model

reduction of more than two orders of magnitude. And yet, the Foster network model gives the same results as the original full CFD model. Figure 9 shows such a comparison. The model order reduction process is handled automatically by ANSYS Simplorer, which uses CFD results as inputs. This model order reduction technology opens the door for simulations that would otherwise have been impractical. For instance, battery thermal control system analysis would benefit from such a fast model.

## Conclusions

The primary concern of electric engineers, is the electric performance of the battery rather than the thermal performance. However, as mentioned before, battery electric performance is a strong function of temperature. So, electric engineers need an accurate and yet simple to use thermal model that couples with their battery electric circuit model. Figure 10 shows such a complete dynamic model.

The complete electric circuit model of a lithium ion battery accounts for non-linear equilibrium potentials, rate and temperature dependencies, thermal effects and response to transient power demand. Traditional thermal network models can also be used to couple with electric circuit models. With the help of VHDL-AMS, which is an IEEE standard hardware simulation language supported by Simplorer, a traditional thermal network model can be generated easily. As a matter of fact, VHDL-AMS can be used for much more complex multiphysics and multi-domain problems, and the John Newman electrochemistry model mentioned above was generated using VHDL-AMS in Simplorer.