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Driving the future of advanced automotive batteries

This white paper describes the methods developed during the computer-aided engineering for batteries (CAEBAT) development project that are now available by using Siemens PLM Software's Simcenter STAR-CCM+™ software and Battery Design Studio™ software. These solutions provide seamless integration between electrochemists and thermal engineers in the battery design process. This project has provided manufacturers like Johnson Controls Inc. (JCI) with world-class technologies to help design innovative battery systems and enable new fuel-saving technologies for vehicles.

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Executive summary

The outcome of the quest to commercialize electric-drive vehicles (EDV) will greatly depend on the cost, lifetime, safety and reliability of the underlying battery technologies. Today, simulation is starting to have a significant impact on bringing viable automotive batteries to market, from integrating small-scale electrochemistry models to system-level modeling of aging, performance and degradation to help fully understand the complete system. This white paper describes the CAEBAT development project that targeted the automotive and lithium-ion battery industries with the goal of driving down development time, and enabling large market penetration of advanced EDV power systems. We talked to Dr. Brian Sisk, director of design analysis for power solutions at JCI, to find out more about the critical role simulation and projects like CAEBAT play in the development of their battery technologies.

Challenges in battery design

Cost, range, charging time, safety, performance and battery life are all difficult hurdles that must be faced to make EDVs commercially appealing and viable. Historically, prototype-driven cell design and qualification testing such as cycle testing (in which cells are subjected to repeated charge-discharge cycles over long periods of time) have been the gold standard for battery design. With a projected life of 10 to 15 years, establishing confidence in the lifespan of the EDV battery is a particularly challenging engineering problem, as it is highly dependent on uncertainties such as varying operating temperatures and environmental conditions.

Sisk manages JCI's global modeling capabilities, including electrochemical, system and vehicle modeling, as well as requirements analysis, vehicle laboratories and analytical laboratories. His team's mission is to support battery and component design engineers by providing an understanding of what their product technologies need to have and identifying new technological opportunities.

"The vehicle battery industry is at a crossroads," Sisk says. "The automotive battery that once needed only to provide starting, lighting and ignition functionality now needs to do more than ever. The battery may be required to support much higher accessory loads, allow complex battery management strategies and provide start-stop operation and even power hybrid or fully electric powertrains."

This rapidly evolving market has spurred a great deal of innovation at JCI, resulting in an increasing breadth of product offerings to address the demands of vehicle manufacturers in terms of cost, size and fuel economy.

Sisk further comments, "We are going to see a proliferation of battery technologies in the market driven by both consumer demand and strong global fuel economy requirements, and simulation plays a critical role in that world."

Impact of simulation

State-of-the-art simulation tools that include flow, thermal and electrochemistry models are now starting to enable the design of EDVs while taking into account the many length scales of the system, including microstructure electrochemistry, detailed cell design, module and pack analysis and overall system design with the battery in-situ.

"Vehicle manufacturers demand flexibility from battery suppliers so they can meet rapidly changing needs and requirements," says Sisk. "Additionally, the strong competition in the battery space means that technical uncertainty can't be solved by over-engineering or providing large margins for error. This environment creates a pace of technological change that simply leaves no time to perform physical experimentation for every requirement and that means simulation is not a luxury. It's an absolute requirement and necessity."

At JCI, the benefits of simulation are enormous and the greatest benefits are often intangible and can be hard to quantify. Sisk notes, "Time is always money, but not all time is created equal. Simulation really shows the benefit when it is the only way to accomplish a task on schedule or to win with a customer with extremely tight time constraints."

It is clear that beyond looking at bottom-line cost savings, companies like JCI consider the true value of simulations by asking questions such as, what business did we win that would have been lost without simulation capabilities?, what project was profitable that would have lost money without simulation?, and what relationships did we save because we were quickly able to perform a simulation in a situation in which experimentation would have been impossible?

The project

In June 2011 CD-adapco, now part of Siemens PLM Software, embarked on a software development project that was co-funded by the Vehicle Technologies office in the U.S. Department of Energy. The origins of the project date back to a request for proposal (RFP) entitled, "Development of Computer Aided Design Tools for Automotive Batteries," which was managed by the National Renewable Energy Laboratory (NREL). This dovetailed with the capabilities of Siemens PLM Software's Simcenter STAR-CCM+, and was used to conduct flow, thermal and electrochemical analysis on lithium-ion pouch cells. The proposal was to enhance the existing capability to apply to all battery cell form factors, specifically the more challenging spirally wound designs.

The team

Taking on this ambitious project required partners who could deliver the necessary technology and validation to demonstrate the value and accuracy of the proposed method. An obvious choice to help with the mathematics and problem definition was CD-adapco's long-term partner in the field of battery analysis, Battery Design LLC. JCI also came on board as they have a broad range of wound cells that are ideal for use as validation cases for such technology. The team was completed with the addition of A123 as their pouch cell was studied to ensure the developed methods worked across all cell shapes.

"Our participation in CAEBAT was extremely beneficial to us," says Sisk. "CAEBAT served to get a wide array of interconnected stakeholders together, including battery manufacturers, software vendors, vehicle manufacturers, academic institutions, national laboratories and government stakeholders. Working together allowed us to align our priorities and to increase the level of fidelity and realism in the available simulation capabilities."

A real benefit for JCI was having their technology, including their specific electrode materials, cells, packs, etc., modeled and validated as part of the research activity undertaken by CAEBAT. That helped to make sure the tools they used were relevant to them. Sisk says, "Increasingly, our focus has been on the battery as a system, not just individual electrodes or cells, and optimizing the system within that context. As a result, the battery chemistry, electronics, thermal design, algorithms and management strategy need to be harmonized. And given that focus, our primary use for CAEBAT is within a systems context, especially for thermal optimization."

The battery modeling process

Figure 1 shows a schematic overview of the different phases of the project.

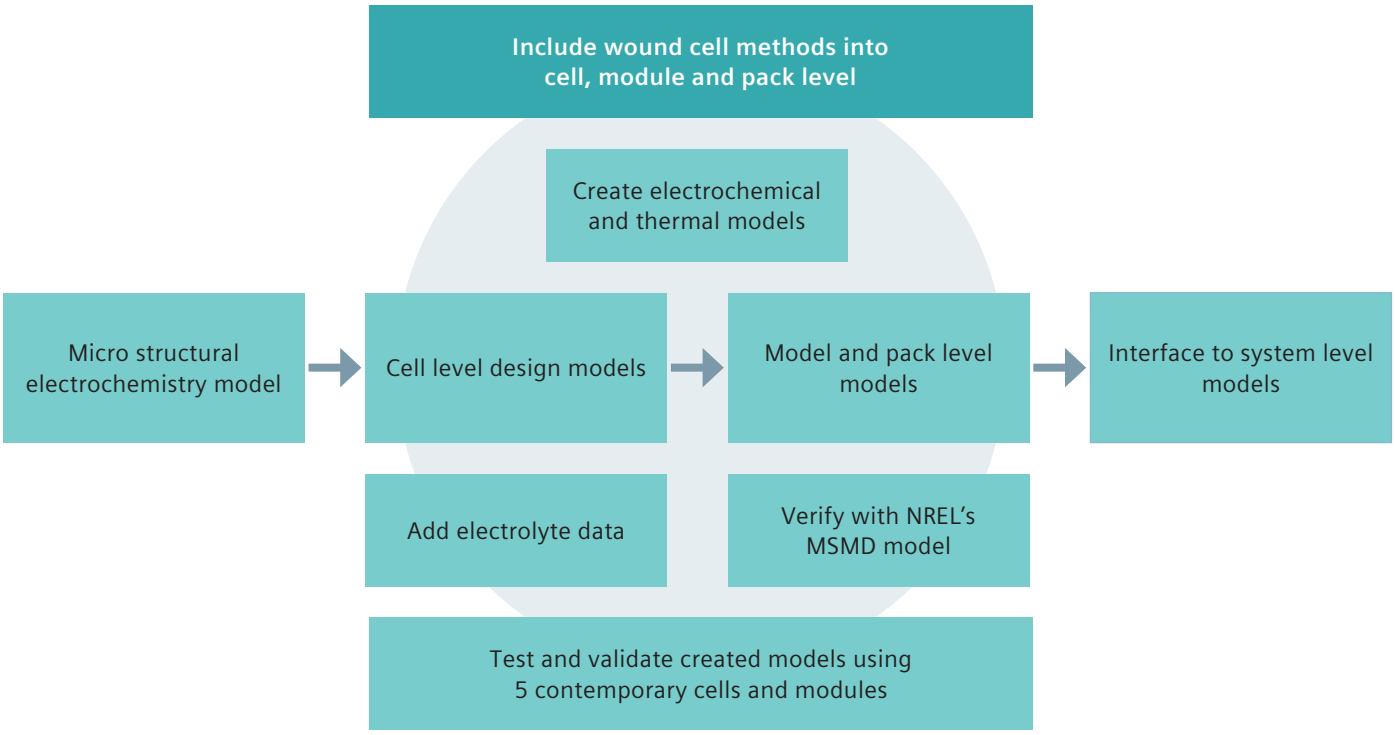


Figure 1: CAEBAT project overview.

The first phase involved detailed software development, producing an industrially relevant and easy-to-use electrochemical and thermal model that can be applied to wound electrode battery types. The resulting simulation technology is applicable both at the cell and module level of analysis, and the fidelity of the model can be controlled by the user depending on their desired output and level of accuracy.

Figure 2 outlines the three steps of the battery modeling process.

Figure 2: Three steps of the battery modeling process.

The process starts with cell data provided by the cell manufacturer, such as the physical dimensions of the cell and its chemical characterization data. This data is used at the cell model level to fine-tune a number of unknown modeling parameters that affect the performance and build of a robust model over the entire temperature, state-of-charge (SOC) and rate range of the cell. An iterative calibration loop is completed to ensure the right balance of all the aspects of the model's performance. Figure 3 shows an example of a result of this calibration process. The voltage prediction is depicted from the cell model (red) versus experimental tests (green) for a 20 Celsius (°C) rate United States Advanced Battery Consortium (USABC) high pulse power characterization at 10 degrees. This is done over the entire temperature, SOC and rate range.

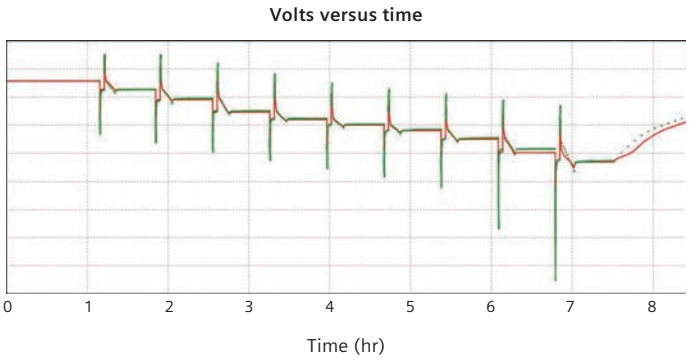


Figure 3: Voltage prediction from the calibrated cell model (red) versus the experimental cell (green).

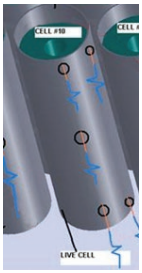
Once an initial model is generated using abstract cell characterization data, it is put to work by predicting a cell's performance using a more realistic drive cycle. These drive cycles tend to feature constantly varying currents or power, and therefore add a level of complexity not seen in the characterization data. These results can be compared with appropriate test work to further validate the model before moving to a three-dimensional representation of the cell in Simcenter STAR-CCM+.

Next, a three-dimensional simulation model is built and the electrodes now have the required high resolution to resolve internal electrochemical and thermal gradients. This not only has an impact on the model run time, but also on the subsequent increase in model fidelity, which is crucial for detailed design. Within the 3D model, each region of the electrode could be operating at a different temperature and hence contributing differently to the cells' electrochemical response. Bringing these together results in an accurate way of predicting the cell's performance in the given cooling system design. Furthermore, using Simcenter STAR-CCM+, the cells can now be stacked or arranged to create a realistic module/pack for further investigation.

Validation and application

During the second phase of the project, five cells from two different manufacturers and spanning three cell shapes (stacked, cylindrical and prismatic wound electrodes) were used to validate the computational model developed using real-world drive cycles at both the cell and module levels.

Figure 4 shows the voltage evolution and temperature resulting from a single JCI VL6P cell analysis during a standard drive cycle. The correlation between analysis (red) and test data (green) shows a good match for voltage prediction. The temperature evolution (blue is analysis, green is test) also indicates an accurate prediction of heat generation in the cell.



Example thermocouple positions

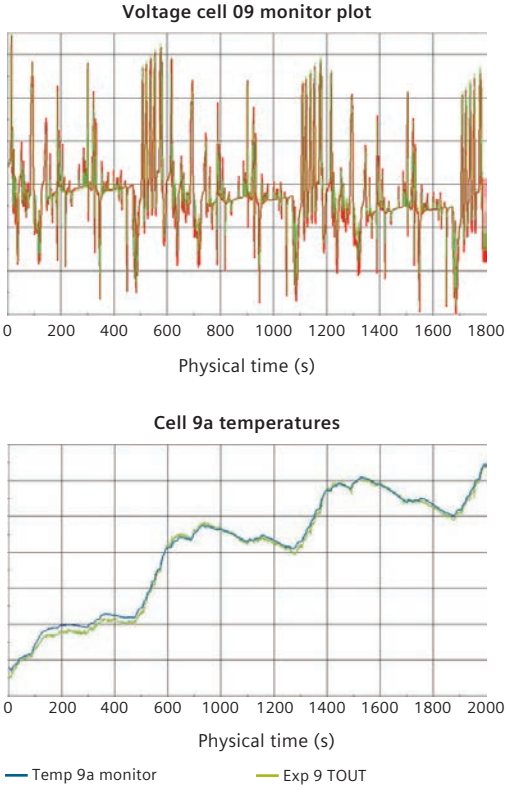


Figure 4: Voltage (analysis in red, test in green) and temperature evolution (analysis in blue, test in green) for a JCI VL6P cell using a standard drive cycle.

Figure 5 shows the simulation results of a module using 12 stacked JCI VL6P cells with a liquid cooling system in between for thermal management. Although this is a much more complex application, the simulations once again capture the experimental trends and the small fluctuations in both the electrical and thermal results. Figure 6 shows the temperature distribution at the end of the 30-minute US06 drive-cycle simulation.

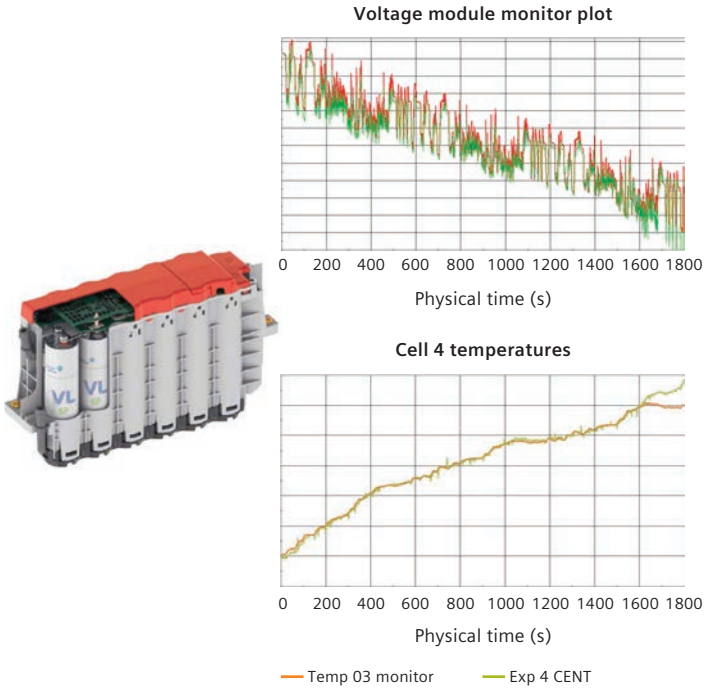


Figure 5: Voltage and temperature for a module containing 12 JCI VL6P cells using a standard drive cycle (analysis in red, test in green).

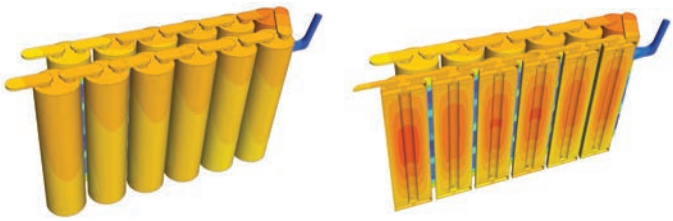


Figure 6: Temperature distribution on surface (left) and on sectional cut (right) for a module containing 12 JCI VL6P cells after 30 minutes of a US06 cycle.

Figures 7 and 8 show additional simulation results, in this case, for a three-cell test fixture. Figure 7 displays the model geometry used for experimental validation of coupled thermal/electrochemical models.

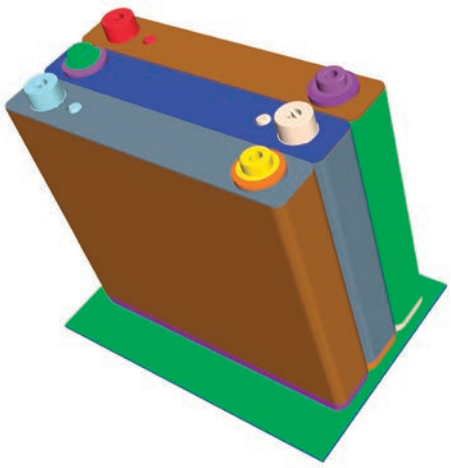


Figure 7: Model geometry (colors for geometric clarity) of a three-cell test fixture used for experimental validation of coupled thermal/electrochemical models.

Figure 8 shows the simulated thermal map after cycling with the highest temperatures shown in red and the lowest in blue.

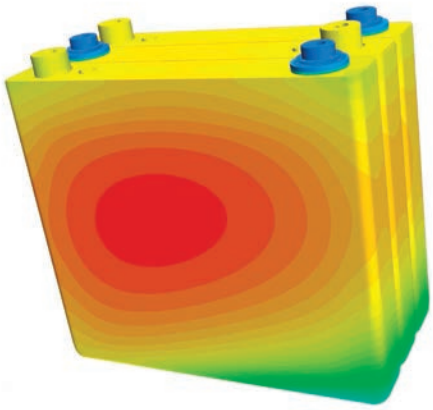


Figure 8: Thermal map after cycling with the highest temperatures in red and the lowest in blue.

To further enhance the simulation methodology, a database featuring 12 contemporary electrolyte formulations typical of those used in modern lithium-ion batteries was added to the software. This enabled a more complete physics-based simulation to take place. Additionally, a complementary calendar aging model was created to work alongside the cell performance models, preconditioning them to the aged state. The approach was also extended into system-level space using either an electrochemical technique or reduced order models. Finally, best practice methods for timely generation of future electrochemical techniques by users were developed and the simulation models were integrated into Simcenter STAR-CCM+ for combined flow, thermal and electrochemical simulation across a range of length scales without redundancy.

Conclusion

The methods developed during the CAEBAT project are now available in Siemens PLM Software's Simcenter STAR-CCM+ and also in the application-specific tool, Battery Design Studio. These solutions provide seamless integration between electrochemists and thermal engineers in the battery design process. By linking the flow, thermal and electrochemical simulations into one environment, a highly accurate solution can be obtained, spanning multiple scales and computational domains from system models to highly resolved complex 3D models. This project has provided battery manufacturers like JCI with world-class technologies to help design innovative battery systems and enable new fuel-saving technologies for vehicles.

Siemens PLM Software

Headquarters
Granite Park One
5800 Granite Parkway
Suite 600
Plano, TX 75024
USA
+1 972 987 3000

Americas
Granite Park One
5800 Granite Parkway
Suite 600
Plano, TX 75024
USA
+1 314 264 8499

Europe
Stephenson House
Sir William Siemens Square
Frimley, Camberley
Surrey, GU16 8QD
+44 (0) 1276 413200

Asia-Pacific
Suites 4301-4302, 43/F
AIA Kowloon Tower,
Landmark East
100 How Ming Street
Kwun Tong, Kowloon
Hong Kong
+852 2230 3308

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