General Electric´s Ecomagination℠ technology is exemplified by the Evolution® Hybrid Locomotive. GE will utilize batteries to help power these locomotives. *Photo courtesy of GE Transportation.*

Modeling Helps Batteries Jump on the Train of Environmental Progress

If all diesel electric locomotives were converted to utilize hybrid technology, a potential projected savings of more than $425 million per year could be realized — using batteries to run freight locomotives makes economic sense. Add this to significant cuts in greenhouse gas emissions and the environmental savings of General Electric's Hybrid Locomotive help move us toward a greener tomorrow. Michael Vallance of GE Global Research is simulating the sodium metal-chloride batteries that will drive GE's hybrid locomotives to enable and even increase these savings.

BY PHIL BYRNE, COMSOL AB

For years, fuel cells had been pushed as the answer for "green" transport even though a commercially viable vehicle was never fully realized. Rather than waiting for a hydrogen economy to be established, hybrid cars such as the Toyota Prius, Ford Escape, Chevrolet Malibu and others have shown that a simpler and better utilization of existing technologies can also lead to substantial improvements in the environmental credentials of a vehicle. Best of all, they're available now.

People have come to learn that such cars, with their repetitive start-stop operation, are an application where hybridized internal combustion/electric drives are more efficient than internal combustion engines alone. But they may not have suspected that a battery-driven electric locomotive would be practical because a train moves heavy loads at fast speeds for long periods and over long distances. Surprisingly, though, batteries can make a substantial contribution, given that they can provide up to 2,000 horsepower to a locomotive.

Recovered Energy Cuts Emissions

"One large difference compared to an automobile is that locomotives spend many minutes while dynamic braking, rather than just seconds. This generates considerable energy that's normally lost," says Michael Vallance. They plan to make use of this energy in their hybrid locomotives to achieve fuel savings of up to 15%, which is equivalent to 25,000 – 30,000 gallons of diesel per vehicle per year, and for eliminating over 300,000 kg of CO_2 emissions – equivalent to that from 2,600 cars. Moreover, the reduction in NO_x emissions is even more significant.

However, GE had to develop an alternate to the lithium and metal-hydride batteries used in passenger vehicles. They needed versions with higher energy densities that can withstand the environment of a long-haul locomotive. Furthermore, these new batteries must be tolerant of cell failures in high-voltage strings, where batteries with failed cells continue to operate safely and effectively.

Figure 1: A locomotive expends considerable energy when braking. In hybrid locomotives, this energy is harnessed and stored by batteries and can be used to supplement energy from the engine. Diagram courtesy of GE Transportation.

How it works

In a conventional locomotive, energy generated by the traction motors (A) during braking is dissipated entirely as heat through resistor grids (B).

In contrast, in a hybrid locomotive, some of that energy is captured in a series of lead-free, rechargeable batteries (C).

The captured energy can then be used to provide power in one of three ways:

- In combination with diesel-electric power (provided by the engine (D) and the electrical system (E)) to consistently deliver the required horsepower.
- As an addition to full diesel-electric power for quick acceleration from a full stop.
- As the primary power source (full battery power).

To develop its own high-temperature sodium metal-chloride battery, GE formed a team spanning its Global R&D laboratories, with members in Niskayuna, NY, USA, Shanghai, PRC and Bangalore, India. This team began a close collaboration with the engineers of GE Transportation in Erie, PA, USA. GE's battery technology has now reached the stage where a full-scale prototype operational locomotive is being shown to potential customers. In fact, back in 2007, GE demonstrated its first hybrid freight locomotive, arriving at Los Angeles' Union Station with CEO Jeff Immelt present.

A Valuable Tip

Michael and his colleagues have since been working with this battery and wanted to better understand the mechanisms that make it function.

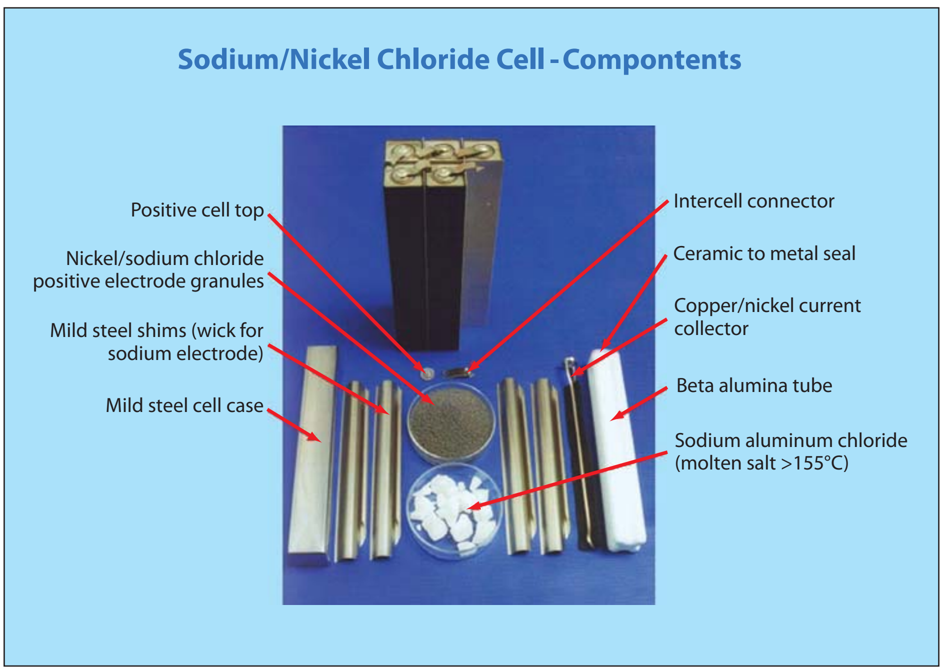

Figure 2: The sodium metal-chloride battery and its components. *Photograph courtesy of GE Transportation.*

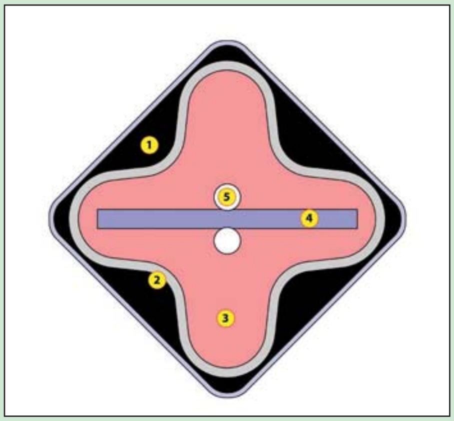

Figure 3. A cross-section of the battery geometry and the various modeling domains:
1. Anode: Molten sodium
2. BASE: Sodium conducting solid electrolyte (β´´ alumina)
3. Cathode: Iron and molten-salt electrolyte (NaCl-saturated sodium tetrachloroaluminate(STCA))
4. STCA Reservoir
5. Cathode current collector

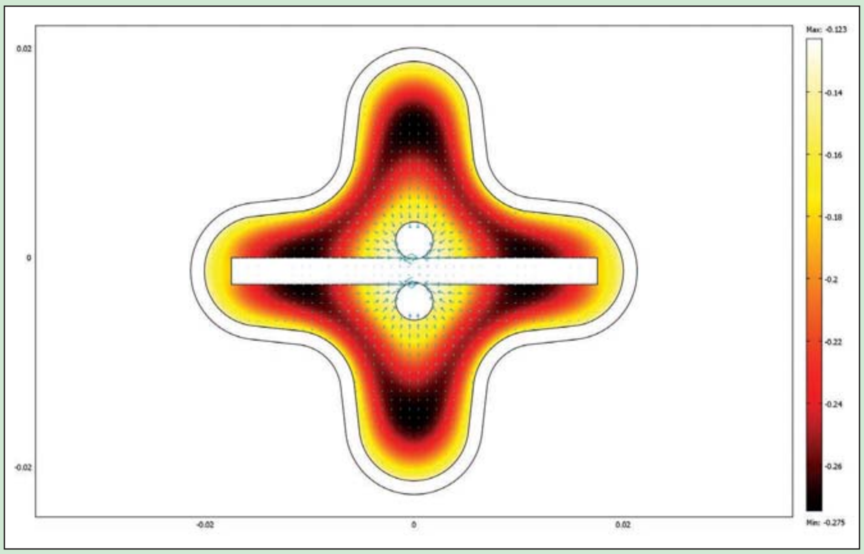

Figure 4: Current density vector and distribution at 58.9% depth of discharge (DoD) in the battery. The arrow plot indicates localized regions of high current density that occur in the area of the connection between the cathode current collector and the STCA reservoir. The color plot indicates the wave front characteristic that the electrochemical reactions undergo within the battery.

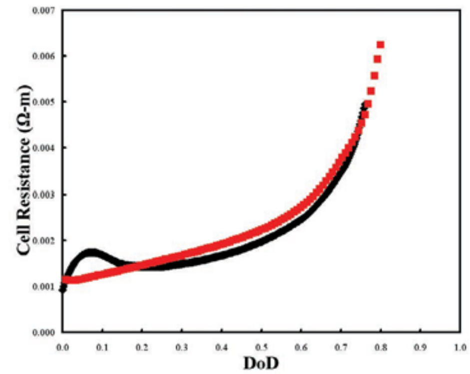

Figure 5: Comparison of experimental results (red points) and the model's prediction (black points) of depth of discharge (DoD) vs cell resistance, which rises significantly after about 60% DoD due to species depletion and transport resistance.

Michael began to look for a modeling software package that was well suited to simulating the electrochemical reactions and material and energy transport that make up the sodium metal-chloride battery. One option raised was the COMSOL Multiphysics software platform. Michael attended a COMSOL Conference in 2007 to learn more about the software. At the conference he also met one of the leading experts in electrochemical simulations, Dr. Ralph E White from the Dept. of Chemical Engineering at the Univ. of South Carolina, who was able to advise him on how to include advanced electrochemical phenomena in his models.

To fully simulate the operational behavior of a sodium metal-chloride battery, you must involve multiple mechanisms. Electrochemical reaction kinetics as described by the Butler-Volmer equations need to be solved at the electrodes, while the model must also consider the transport of ions to these electrodes through migration, diffusion and convection. A number of participating materials change phase as a part of the battery's charging or discharging operations, and the corresponding kinetics must also be factored in. Furthermore, temperature plays an important role in many of the battery's physical characteristics including ionic mobility and the species' phases, so operational temperatures must be held within a narrow range.

Considering all of these factors, COMSOL Multiphysics' ability to couple them and solve them simultaneously is a key feature. The software was used to develop an accurate, realistic battery model.

Understanding Leads to Design Changes

The models he has created have uncovered results that led to a heightened understanding of the battery. In the present version of the battery, the modelers have been able to identify areas of high current density, and this information was used to adjust manufacturing tolerances at critical regions. The model provided additional insights concerning convective flows in the cathode, which lead to an experimental investigation of modified geometries.

The value of modeling even extends into operating issues. Plotting cell resistance versus depth of discharge (DoD – the extent to which the reacting materials in the battery are consumed) indicates when operators should start a recharging cycle. Because cell resistance starts to rise exponentially after about 60% DoD, a battery should not be discharged long beyond this point.

COMSOL Multiphysics will further be useful for investigating other properties such as the battery's structural integrity due to vibrations and other duress it experiences in the locomotive. ■