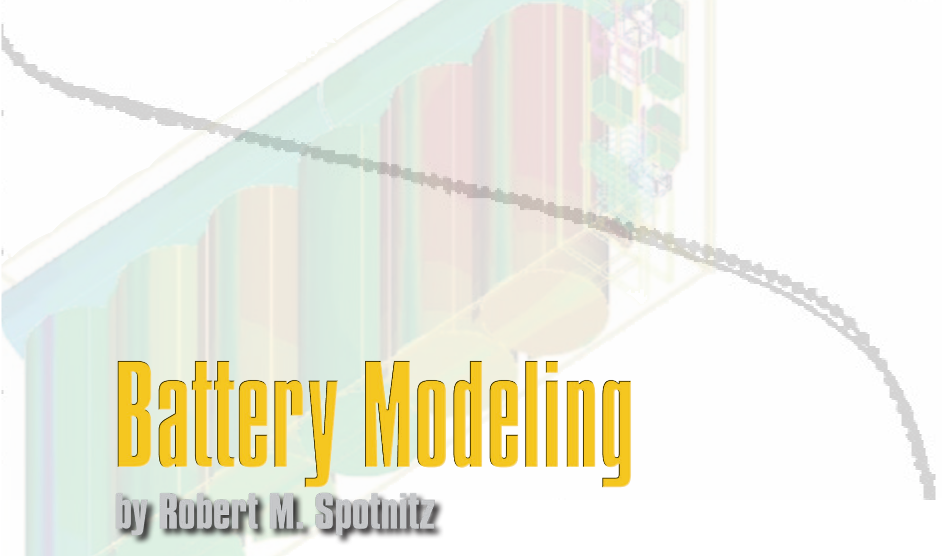

Battery Modeling

by Robert M. Spotnitz

Battery modeling, or the mathematical description of batteries, long considered an academic pastime, now plays an important role in the design and use of batteries. The field of battery modeling can be divided into the following two areas.

1. *Estimation of battery performance.* Given an already constructed battery, the problem is to estimate how that battery will perform under specific conditions of interest to the user of the battery. This problem is typically addressed by testing batteries under the specific conditions of interest and using a model to represent the test results. Approaches for representing test results range from simple statistical models to neural nets to complex, physics-based models. Basing the model on test data becomes problematical when testing becomes impractical (such as a 10-20 year life test). Real-time estimation of battery performance, an important problem in automotive applications, falls into this area.

2. *Battery design.* Here the problem is to estimate how the design of a battery impacts its performance. This is a difficult problem and can be only partly addressed because the complexity of most battery systems defies characterization. Our inability to characterize the mechanisms involved in many battery chemistries limits the application of modeling to battery design. Instead, battery design relies heavily on the tried and true approach of build and test rather than on engineering principles. This build and test approach is practical because test cells are often inexpensive to build and key tests often can be carried out rapidly. In the short term, developing a battery by trial and error actually takes less time than determining how a battery works and using that mechanistic understanding for design. However, those aspects of battery operation that are understood well enough to model such as temperature and current distribution have undergone significant optimization. Such advances indicate that as our understanding of batteries increases and more aspects of battery operation become amenable to modeling, we may expect a dramatic acceleration in the pace of battery development.

The area of battery performance estimation receives much more attention than the area of battery design. Battery performance can be estimated by a wide range of workers while the area of battery design is limited mostly to battery developers. Battery developers consider design information highly proprietary and are reluctant to divulge such information to model developers, who, for the most part, still tend to be academics.[1-5] Recently available, third-party battery design software provides some standard designs that can be studied openly and so promotes development of the science of battery design. However, progress in the area of battery design has benefited most by the advent of lithium-ion batteries.

Lithium-ion or rocking-chair batteries are the newest and have the most well-understood battery chemistry. Both the positive and negative electrodes serve simply as hosts for lithium ions that transport through a binary electrolyte. This system can be readily modeled. For example, a recent paper[6] by a battery developer shows that a physics-based model can provide a remarkably accurate estimate of battery behavior (see Fig. 1). This understanding of lithium-ion batteries has encouraged modelers to develop successful methodologies for design of charge/discharge performance[7,8] and abuse tolerance.[9,10]

Even further, materials researchers now use molecular or computational modeling[11] to aid in the design of materials ranging from active materials to electrolytes. The integration of molecular models for materials with continuum models for batteries falls into the area of multiscale modeling,[12] but is not be discussed here.

This article highlights some major applications of battery modeling in the areas of performance and design, and describes recent developments aimed at making modeling more accessible to battery developers and users.

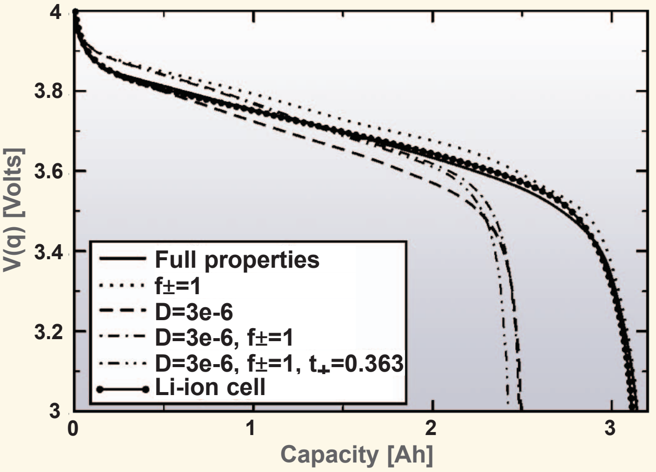

FIG. 1. *Comparison of simulated discharge curve to experimental discharge curve for a Li-ion cell.*[6]

Batteries for Hybrid-Electric Vehicles (HEV)

HEVs like the Toyota Prius or Ford Escape rely on the battery to provide power for acceleration and recover some energy from regenerative braking. For the battery to be ready to either accept or deliver energy, it must be at some intermediate state-of-charge (SOC), perhaps 50%, so determining and controlling SOC is critically important. Researchers

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at GM have described a particularly elegant way for real-time SOC estimation.[13]

One may think that current integration will provide a good estimate of SOC. However, the nickel metal hydride (Ni/MH) batteries used in HEVs tend to lose charge during rest periods, and the current efficiency on charge can be less than 100%. To correct for these effects, the SOC may be estimated by dynamically fitting measured voltage and current data to a model. This model-based SOC estimate may be averaged with a SOC estimate obtained by current integration to give an accurate SOC estimate over a wide range of conditions. A side benefit of this approach is that one model parameter, a series resistance, gives an indication of the state-of-health of the battery.

Another important aspect of HEV battery design is temperature uniformity. Nonuniform temperature distributions lead to shorter life because the hot areas wear out faster than the cool areas. HEV batteries typically consist of many cells in series. The current flows into each cell through a post and is then distributed along a grid or plate. This situation can cause the grid near the post to become much warmer than the grid furthest away from the post. Mathematical modeling work by Pesaran *et al.*[14] shows that the 2001 model Ni/MH module in the Toyota Prius suffered from a non-uniform temperature distribution while the 2004 model, that used two connections for each grid, had a nearly uniform temperature distribution (Fig. 2). The model results were verified by thermal imaging experiments.

Batteries for Portable Computers

As in HEVs, a uniform temperature distribution is important in battery packs for portable computers to provide long life. Maleki and Shamsuri[15] modeled the temperature distribution in a laptop computer battery pack (see Fig. 3). Interestingly, they found that the neighboring electronic circuit strongly influenced the temperature distribution. This analysis suggests that insulating the cells from the electronics may improve thermal uniformity.

The problem of SOC estimation is also important in portable computers to give users an indication of available runtime. The usable capacity of a lithium-ion battery can be estimated using a simple model

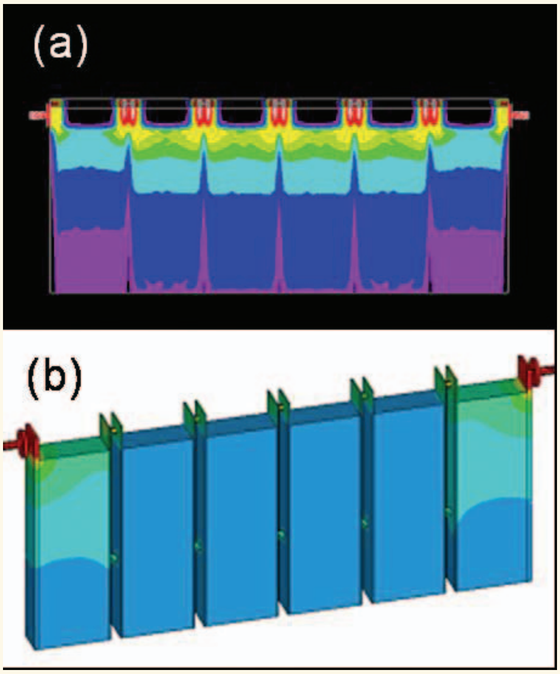

Fig. 2. *Computed temperature distributions for Ni/MH modules containing (a) one post for electrode and (b) two posts for each electrode.*[14]

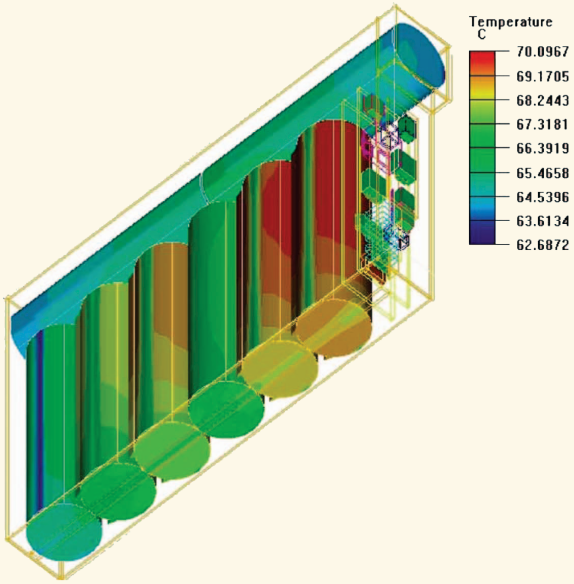

Fig. 3. *Computed temperature distribution in a battery pack for portable computers.*[15]

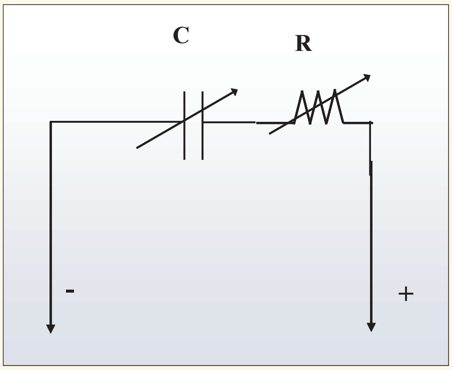

Fig. 4. *Simple circuit model for lithium-ion battery.*

like that depicted in Fig. 4. The model involves two parameters: *Ro* and *Vo*. *Vo* is the open-circuit voltage of the battery and is an accurate indicator of SOC for lithium-ion batteries. *Vo* is determined when the battery is at rest and updated during charge or discharge of the battery by coulomb counting. *Ro* is the impedance of the battery and is dynamically obtained by real-time impedance measurements. For notebook computers, this approach appears to give remarkably accurate estimates of battery capacity and is used in a chip provided by Texas Instruments.[16]

Uninterruptible Power Supplies (UPS)

Many businesses that rely on computers, such as stockbrokers, rely on UPS systems to avoid even momentary interruptions in electrical service. Assessing the state-of-health of UPS batteries is of great importance to such businesses. A promising model-based approach[17] involves use of a model that accounts for electrode kinetics, active surface area of the electrodes, liquid-phase mass transfer (concentration and potential gradients in solution), and solid-phase ohmic drops. Some key parameters (thickness of electrodes and separator, tortuosity of electrodes) for this complex model can be fit to an experimental charge/discharge curve. Then the calibrated simulation model may be used to estimate the capability of the battery to perform its UPS function. The model calibration procedure may be automated and carried out on a regular schedule so that the health of the battery may be monitored.

The life of lead-acid batteries is often limited by corrosion of the positive grid. The lead grid is coated with positive active material (PAM). If the grid oxidizes, then there is less lead available to carry current and this may lead to eventual failure of the battery. Ball *et al.*[18] provided insight into the problem by computing the current density distribution around a grid bar. They correlated the computed current density with corrosion observed on a grid (Fig. 5). Areas of high current density corresponded to areas of high corrosion. This approach points the way to more corrosion-resistant grids and thus longer-life batteries.

Aerospace Batteries

In aerospace applications, batteries may sit for years before being used, so there is a need to estimate any detrimental effect aging has on battery capacity. Lithium-ion batteries undergo irreversible capacity loss when stored for long periods of time. At cell voltages below 4.0 V, the major source of capacity loss during storage is self-discharge of the negative electrode. Broussely[19] has used a film-growth model to describe this process successfully. The self-discharge reaction produces a film that inhibits further self-discharge, so the process is self-limiting. The rate of film growth is inversely proportional to thickness (so grows according to the square root of time) and the rate constant follows Arrhenius behavior. Plots of irreversible capacity loss *vs.* the square root of time are linear, and the slopes of such plots obtained at temperatures below 50°C follow an Arrhenius expression. This behavior provides confidence in extrapolating measurements made over 1-2 years to 5-10 years.

Software for Battery Modeling

Professor John Newman provides a model for lithium and lithium-ion batteries on his website.[20] Most battery modeling is carried out using general-purpose tools such as MATLAB® and ANSYS®. However, the growing importance of battery modeling has led to the development of customized software. The most comprehensive approach to battery design and simulation is provided by the Battery Design Studio® software offered by Battery Design.[21] The software is primarily a user interface for accessing battery models, and provides a user friendly environment for battery design and simulation as well as analysis of battery data. The software includes sizing routines for various cell geometries (stacked or spirally wound), models for simulating battery behavior, including abuse, a database, and tools for visualizing and analyzing battery data. These features constitute a standardized means to communicate battery information (designs, data, and models) among interested parties.

The capability to communicate battery information easily using software makes modeling more accessible to battery developers, and makes battery design and performance information more accessible to modelers. By facilitating comparisons between model predictions and data, such software brings the full force of the scientific method to bear on the problem of battery design.

Final Remarks

Mathematical modeling is firmly entrenched for estimating battery performance as evidenced by the applications discussed above. Mathematical modeling is only beginning to impact battery development. The overwhelming complexity of battery systems encourages battery developers to focus their resources on building and testing batteries rather than developing mathematical models. However, modeling is now more accessible to battery developers thanks to third-party software. Battery developers should strive to make battery design part of the design process of battery-powered products.

To paraphrase a recent statement, "You go to production with the battery you have, not the battery you want." Producers of battery-powered devices must use whatever batteries are available in their products because designing a custom battery takes too long. Reducing the design cycle of a battery from years to months will

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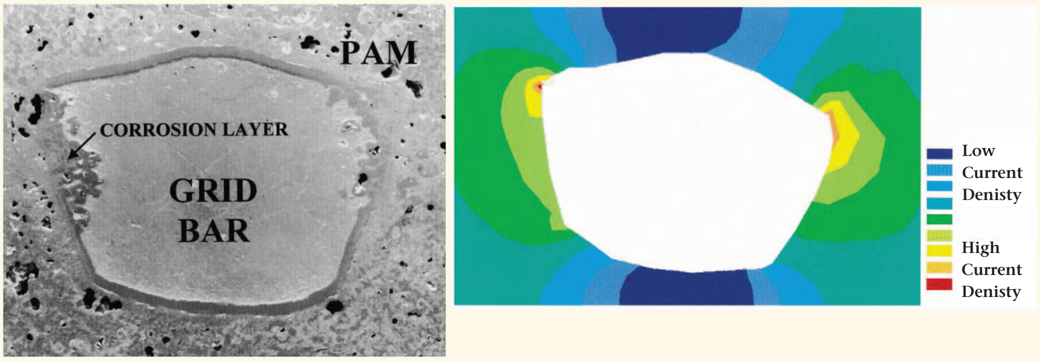

Fig. 5. *Computed current distribution on lead-acid battery grid and electron micrograph cross section of actual grid.*[18]

enable customization of batteries for individual products, making battery-powered products more useful and batteries more valuable. Modeling is the most proven method for shortening design cycles. Making battery modeling an integral part of the battery design process is the battery industry's biggest challenge. ■

References

1. T. F. Fuller, M. Doyle, and J. Newman, *J. Electrochem. Soc.*, **141**, 1 (1994).
2. D. Fan and R. White, *J. Electrochem. Soc.*, **138**, 18 (1991).
3. C. Y. Mak, H. Y. Cheh, G. S. Kelsey, and P. Chalilpoyil, *J. Electrochem. Soc.*, **138**, 1607 (1991).
4. C. Y. Wang, W. B. Gu, and B. Y. Liaw, *J. Electrochem. Soc.*, **145**, 3407 (1998).
5. N. Harb and R. M LaFollette, *J. Electrochem. Soc.*, **146**, 809 (1999).
6. L. O. Valøen and J. N. Reimers, *J. Electrochem. Soc.*, **152**, A882 (2005).
7. T. F. Fuller, M. Doyle, and J. Newman, *J. Electrochem. Soc.*, **141**, 982 (1994).
8. M. Doyle and Y. Fuentes, *J. Electrochem. Soc.*, **150**, A706 (2003).
9. T. D. Hatchard, D. D. MacNeil, A. Basu, and J. R. Dahn, *J. Electrochem. Soc.*, **148**, A755 (2001).
10. E. Roth, D. Doughty, and R. M. Spotnitz, Paper 1302 presented at the Quebec City, Canada, Meeting of The Electrochemical Society, May 15-20, 2005.
11. G. Cedar, M. Doyle, P. Arora, and Y. Fuentes, *MRS Bull.*, **27**, 619 (2002).
12. See papers from symposium on *Multiscale Simulations of Electrochemical Systems*, presented at The Electrochemical Society Meeting, Los Angeles, CA, Oct. 16-21, 2005.
13. M. Verbrugge and E. Tate, *J. Power Sources*, **126**, 236 (2004).
14. A. Pesaran, A. Vlahinos, D. Bharathan, G.-H. Kim, and T. Duong, Paper presented at 21st Electric Vehicle Symposium, Monaco, April 4-7, 2005.
15. H. Maleki and A. K. Shamsuri, *J. Power Sources*, **115**, 131 (2003).
16. Y. Barsukov, in *Advances In Battery Charging, Monitoring, and Testing*, August 19, 2004, Conference Proceedings, Denver, CO.
17. A. Tenno, R. Tenno, and T. Suntio, *J. Power Sources*, **103**, 42 (2001); A. Tenno, R. Tenno, and T. Suntio, *J. Power Sources*, **111**, 65 (2002).
18. R. J. Ball, R. Evans, and R. Stevens, *J. Power Sources*, **103**, 213 (2002).
19. M. Broussely, in *Advances in Lithium-Ion Batteries*, W. A. van Schalkwijk and B. Scrosati, Editors, Kluwer Academic/Plenum, New York (2002).
20. http://www.cchem.berkeley.edu/~jsngrp/fortran.html
21. http://www.batdesign.com/

About the Author

Robert Spotnitz *is President of Battery Design LLC in Pleasanton, California where he develops software for battery design and simulation. He teaches short courses on battery design for ECS and the Advanced Automotive Battery Conference. He can be reached at rspotnitz@batdesign.com.*