INL chemical engineer Kevin Gering developed the Advanced Electrolyte Model to guide testing of new battery chemistries such as these Li-ion cells.

INL Advanced Electrolyte Model: Virtual Laboratory for Tomorrow's Electrolyte Systems

By Kortny Rolston, *INL Communications & Governmental Affairs*

When Doug Brune began developing a new battery electrolyte, the Dow Chemical researcher faced months of conducting experiments to find the right combination of solvents.

Instead, he called Kevin Gering at Idaho National Laboratory.

Brune had heard Gering speak at a conference about his Advanced Electrolyte Model (AEM), a powerful tool that analyzes and identifies potential electrolytes for battery systems.

"As soon as this project came up, I contacted (Gering)," Brune said. "We needed to identify some co-solvents that would help improve the transport properties of the solvent mixture we wanted to use and needed to do it quickly. We thought (AEM) could help us."

It did.

Brune provided Gering with the properties they were looking for in co-solvents, information about the lithium-ion battery for which the electrolyte was being developed and other specifications.

Gering fed the information into the AEM, which predicts and reports key transport and thermodynamic properties and how electrolytes behave in the electrochemical cell environment.

Within a few weeks, the model produced reports that identified the best compositions of electrolytes, preferred solvents for battery use, and a suite of properties from molecular-scale ion solvation quantities to macro-scale transport properties.

The Advanced Electrolyte Model reduced the number of experiments scientists need to perform on experimental electrolytes for batteries.

"The (AEM) narrowed down our choices and identified solvents we hadn't considered," Brune said. "The model saved us a lot of time. Without it, we would have conducted at least 1,000 experiments and only solvents we thought would work. With Kevin's model, we only ran about 300 experiments and were able to test a wider range of solvents."

Why electrolytes?

For a battery to work, it needs a conductive medium to act as a bridge and carry ions from the anode to cathode and back again. That medium is known as an electrolyte — a substance that produces ions when a salt is dissolved in solvents.

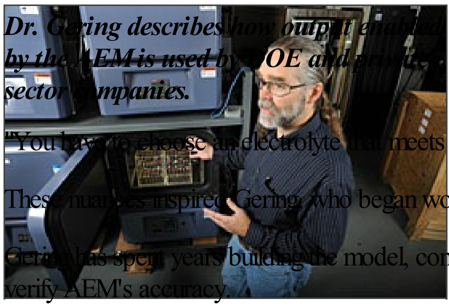
"Electrolytes are center stage for how well batteries work," Gering said. "Choosing the right electrolyte makes a tremendous difference in battery performance and the life of the battery."

However, there is no one-size-fits-all approach to battery electrolytes.

Researchers consider several factors, including battery material, what it will be used for, the range of conditions in which the battery will operate and its expected service life.

Take electric-drive vehicles and today's "smart" phones.

Both are powered by rechargeable lithium ion batteries. But they contain different electrolytes because of the demand on the battery.



Dr. Gering describes how output enabled by the AEM is used by DOE and private sector companies.

An electric vehicle has periods of high demand and must operate in different temperatures that vary daily and throughout the year — a factor that influences battery life. A cell phone battery operates in more predictable conditions.

"You have to choose an electrolyte that meets the demands of the application," Gering said.

These nuances inspired Gering, who began working with electrolytes while pursuing his Ph.D., to build the AEM.

Gering has spent years building the model, constructing the mathematical framework, inputting data on various electrolytes and running tests to verify AEM's accuracy.

Gering and others have investigated a multitude of different electrolyte systems with the model. To date, the model's average accuracies are within 5 percent deviation or less for metrics like conductivity. The tool even detected errant lab data for one of Gering's customers.

How does AEM work?

The model functions as a virtual lab and simulates experimental conditions to produce an exhaustive set of results. It acts like an "electrolytes genome," putting its finger on the DNA of why electrolytes behave as they do.

The underpinnings of the model are a comprehensive set of mathematical expressions that describe the statistical mechanics or chemical physics of electrolytes. AEM captures the molecular interactions between all the electrolyte species, which impact measured properties important to battery applications and beyond.

Researchers provide Gering with specifications about the project, a batteries' intended use and other parameters. AEM then "runs" experiments and refines the list of potential electrolytes, producing reports on properties and a detailed optimization based on several key factors.

This has become increasingly important since many of today's advanced batteries contain complex, multiple-solvent electrolyte systems. AEM routinely evaluates properties for such electrolytes that typically contain up to five solvents and two salts each.

To Brune, that is what sets the AEM apart from other models.

"There are models out there that look at viscosity or conductivity or other individual electrolyte factors, but I haven't seen any others like (Kevin's)," Brune said. "His does it all."

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