Dr. Kevin Gering inspects coin cells used for electrolyte studies at Idaho National Laboratory. The AEM guides rapid, yet thorough, investigation of candidate electrolyte systems.

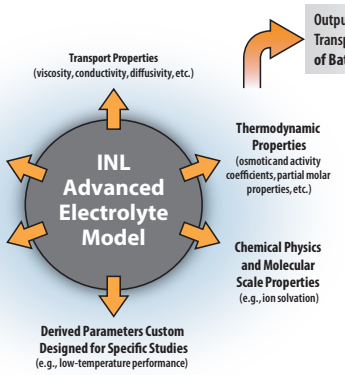
Advanced Electrolyte Model (AEM)

Software predicts battery electrolyte solution interactions

Technological Marketing Summary

Alessandro Volta introduced the voltaic pile in 1800, ushering in the age of portable power and kicking off a relentless pursuit of a better battery that continues unabated today. A far cry from crude stacks of copper and zinc plates separated by brine-soaked paper, today's batteries are marvels of modern engineering that utilize exotic materials in novel configurations.

Containing a complex mixture of chemical elements in its four primary working components (the cathode, anode, separator, and electrolyte solution), effective batteries are limited to key combinations within the periodic table that represent the best levels of performance, value, safety, and environmental impact. While the possible combinations are finite, small tweaks to their relative proportions can produce fundamentally different properties. Developing new and improved battery configurations using traditional methods is a time-consuming and expensive process.



Looking to overcome this, researchers at Idaho National Laboratory have developed sophisticated modeling software that quickly and accurately assesses both macro-scale effects and molecular level interactions of electrolytic solutions, analyzing and reporting on more than 35 key parameters. The Advanced Electrolyte Model (AEM) can handle multicomponent solutions and can be run on a laptop computer, delivering results orders of magnitude faster than competing technologies. The resulting modeled predictions have been experimentally verified to be within a 5- to 10-percent deviation of lab data, often less.

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The Energy of Innovation

Idaho National Laboratory

Ab initio vs. Chemical Physics Models

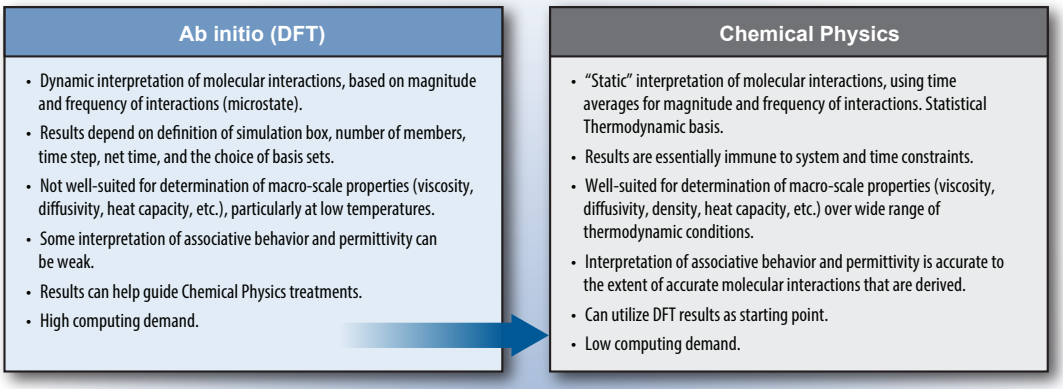

Figure 1. Chemical Physics approaches, such as the Non-Primitive Associative form of the Mean Spherical Approximation (NPAMSA), offer significant advantages in streamlining the computational process, while yielding a wide array of accurate property predictions in a fraction of the time required by ab initio models (density functional theory – DFT).

For more information

Technical Contact:

Kevin Gering

kevin.gering@inl.gov
208-526-4173

Communication Contact:

Nicole Stricker

nicole.stricker@inl.gov
208-526-5955

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The result is a faster and less expensive workflow, one that is highly accurate, responsive to a user's specific needs, and applicable to real-world scenarios. The technology won an R&D 100 Award in 2014, has been successfully utilized by Dow Chemical Company, Xalt Energy and others, and was recently licensed by Dalhousie University for its work on high-tech battery development.

Technology Description

At the heart of every battery is the electrolyte (salts dissolved in a solution), the material responsible for transporting electrically charged ions across the two electrodes and allowing flow of electricity in the process. Modern battery electrolytes are composed of numerous solvents and salts, in ratios specific to their intended usage: A battery designed for robust cold weather output will be designed differently than one designed for, say, rapid recharging, even if the chemicals involved are identical. The AEM can analyze systems with multiple solvents and dual salts to find optimum values of chosen parameters such as conductivity, diffusivity, and ion desolvation energy, removing the guesswork about an electrolyte's qualifications for a specific application. And since batteries can experience wide changes of internal and external conditions, the AEM provides evaluations of electrolyte properties over wide ranges of temperature, salt concentration and solvent composition. Much quicker than quantum chemical methods of electrolyte analysis, density functional theory (DFT), and molecular dynamics (MD), the AEM provides robust predictions without having to depend on step-by-step simulations along a timeline. This results in a model that reduces required lab work and allows for rapid exploration of new components, configurations, and usage conditions.

Technological Benefits

For any given usage scenario, a battery is judged on its safety, longevity, energy density (the amount of energy it can store compared to its weight), how reliably and steadily it discharges, how quickly it can be recharged, how many times it can be recharged, its environmental impact, and, of course, its cost to the consumer. Virtually all these metrics have a connection to the chosen electrolyte formulation. Small tweaks identified by the AEM to existing battery chemistry can alter any of these variables, resulting in an improved battery for a given application.

Potential Applications

More than just a tool to find a superior battery, the AEM can be used to improve any electrolytic application, from petroleum and gasoline refining to large-scale water processing and desalination projects. It can even be used in medical research to better understand the role of electrolyte composition in the human body's own metabolic functions.