

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



Advanced Electrolyte Model

Genome-level Investigation for Industry

Mapping the human genome has advanced our understanding of life, health and cures for diseases. Many technologies could benefit from ‘genome-level investigations.’

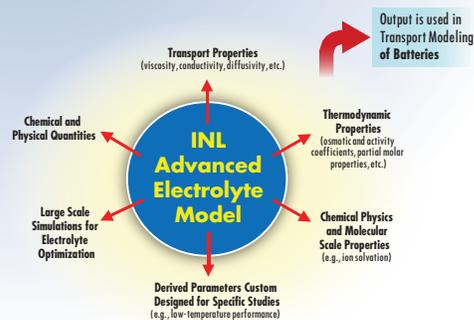
Now, a ‘disruptive, virtual scientific simulation tool’ that delivers a genome-level investigation for electrolytes is available. Idaho National Laboratory researcher Dr. Kevin Gering has developed the Advanced Electrolyte Model (AEM), a copyrighted, molecular-based, scientifically proven simulation tool.

AEM revolutionizes electrolyte selection, optimizing material combinations and key design elements to make battery design and experimentation quick, accurate and responsive to specific needs. AEM predicts and catalogs premier electrolyte metrics, evaluating and comparing more than 35 parameters to recommend optimal solutions. The AEM lets scientists and engineers “look under the hood” of

highly complex electrolyte systems, to gain deeper understanding of what vitally contributes to a multitude of electrolyte properties, then use this knowledge to design better systems. The computationally-streamlined AEM accelerates our acquisition of scientific knowledge toward real applications.

Gering’s AEM proved its value in aiding the Dow Chemical Company in developing a new battery electrolyte. Dow’s Doug Brune said, “The (AEM) narrowed down our choices and identified solvents we hadn’t considered” and “the model saved us a lot of time” (e.g. reduced experimental measurements from 1,000 to 300).

When used as a scientific tool for battery developers, AEM explores and reports with certainty and clarity on



molecular-to-macroscale level aspects of electrolyte behavior, removing the guesswork about qualification of an electrolyte for specific applications.

AEM reduces lab work and permits rapid exploration of other components configurations and usage conditions, as proven in DOE’s Computer Aided Engineering of Batteries program and Argonne National Laboratory’s lithium-ion investigations.

Other potential applications include water processing and chemistry of desalination and distillation, medical research perusing electrolytic functions

Continued next page

The Energy of Innovation



Continued from previous page

in human cells, energy systems (petroleum and gas refining), crystallization processes, ion exchange systems, and more.

AEM is a scientific modeling tool capable of exploring activity at the molecular level to simulate, diagnose and predict electrolyte behaviors and interactions, and the properties that emanate from them. AEM disrupts current electrolyte knowledge and design, while serving as a force multiplier for industry.

Technical Discussion

AEM employs a “static model” approach for each unique condition that enables a computational route that is orders of magnitude faster than ab initio techniques of density functional theory (DFT) and molecular dynamics (MD) techniques (see Figure 1), with no loss of accuracy to the outputs. In a static model, aspects of key interactions such as ion solvation are defined through time averages that incorporate solvent residence times around ions and configuration-dependent distance-of-approach of solvents to ions. Consequently, AEM works quickly and seamlessly over vast ranges of solvent

composition, salt concentration, temperature, and permittivity domains to provide robust predictions. Contrast that to DFT/MD, which depend on step-wise simulations along a timeline to achieve information that parallels AEM’s time averages. For a single condition at lower temperatures, DFT and MD can require more than an hour to complete a rudimentary simulation with very limited output, but AEM is able to predict the substance of key outputs for several thousand distinct conditions within that same timeframe. While Figure 1 indicates that chemical physics models can use some information from the ab initio models, they don’t depend on them.

AEM analyzes and reports on more than 35 key selected parameters. Some of those include Solvated Ion Sizes, Solvent-to-ion Binding Energies, Solvation Numbers, Ion Desolvation Energies, Density, Viscosity, Osmotic coefficient, Conductivity, Diffusivity, Ion Hopping, Communal Solvation and more.

Comparisons

The Advanced Electrolyte Model (AEM) far exceeds its competitors in analyzing and characterizing electrolytes and

component materials and combinations, as well as recommending optimal solutions toward specified requirements. In each comparison category, AEM offers key advantages compared to DFT, Industrial Process/Waste Stream Simulators (IPWSS) and Physical Data Collection (e.g. empirical analysis).

AEM has applicability across many systems due to its generalized molecular scale basis, which makes it independent of any one application. Additionally, it is the only tool of its type developed specifically to support battery electrolyte systems, a major area of interest to those working in electrolyte design and manufacture.

In consideration of these comparisons, AEM offers the potential of lower operating and capital costs, higher accuracy and speed far beyond the capacity of its competitors. These improvements make it a ‘heads and shoulders’ preferred model to others.

Battery Design Studio President Robert Spotnitz said AEM “has simplified the design process for lithium-ion batteries which are used in many markets, including consumer, aerospace, military and automotive.” Video available at www.inl.gov/aem

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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).

Ab initio (DFT)	Chemical Physics
<ul style="list-style-type: none"> • Dynamic interpretation of molecular interactions, based on magnitude and frequency of interactions (microstate). • Results depend on definition of simulation box, number of members, time step, net time, and the choice of basis sets. • Not well suited for determination of macro-scale properties (viscosity, diffusivity, heat capacity, etc.), particularly at low temperatures. • Some interpretation of associative behavior and permittivity can be weak. • Results can help guide Chemical Physics treatments. • High computing demand. 	<ul style="list-style-type: none"> • “Static” interpretation of molecular interactions, using time averages for magnitude and frequency of interactions. Statistical Thermodynamic basis. • Results are essentially immune to system and time constraints. • Well suited for determination of macro-scale properties (viscosity, diffusivity, density, heat capacity, etc.) over wide range of thermodynamic conditions. • Interpretation of associative behavior and permittivity is accurate to the extent of accurate molecular interactions that are derived. • Can utilize DFT results as starting point. • Low computing demand.