

# AEM™

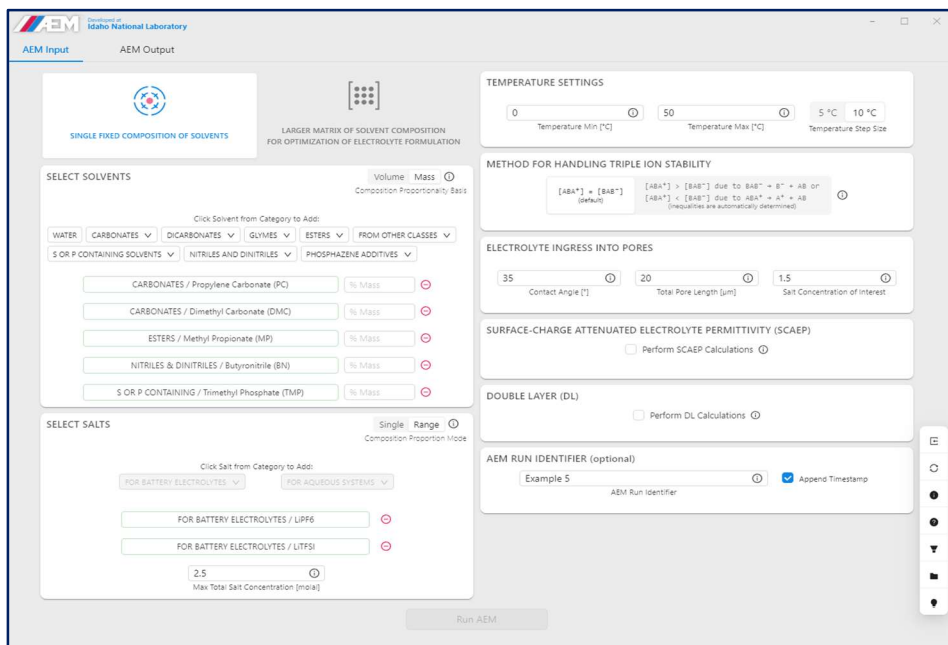
## The Advanced Electrolyte Model

### Features and Benefits

- **Molecular-level Predictions:** Cutting-edge software specializing in molecule-based chemical physics property predictions for electrolyte solutions. It plays a pivotal role in screening and optimizing battery electrolytes.
- **Performance Optimization:** Focused on resolving critical issues such as understanding double-layer behavior, lithium desolvation, and assessing field effects on solvents within the Solid Electrolyte Interface (SEI).
- **Multi-Solvent Compatibility:** Excels in accurately predicting properties for multi-solvent systems (up to 5 solvents or more) and two-salt systems. This versatility enables comprehensive exploration of complex electrolyte combinations.
- **Diverse Component Database:** The AEM Component Database boasts an extensive collection of electrolyte components, which is continuously expanding. It currently encompasses 60 solvents and nearly 40 salts, with ongoing updates and additions.

### GENERAL DESCRIPTION

The Advanced Electrolyte Model (AEM) developed by Dr. Kevin Gering at Idaho National Laboratory (INL) and exclusively available through Ridgetop Group, is an innovative molecular simulation tool that revolutionizes electrolyte chemistry optimization. With over 100 property metrics generated in each run, it effectively acts as a virtual laboratory for exploring genome-level properties. AEM's extensive database encompasses more than 60 solvents and near 40 salts, offering users a wealth of options while considering the consequences of their selections.



**The AEM™ Graphical User Interface (GUI)**

Its scientific foundation is grounded in the Nonprimitive, Nonrestricted Associated form of the Mean Spherical Approximation (NPNRAMSA), further enhanced by an ion-solvation equation of state (IS-EOS) for precision in predictions. Predictions for many systems have average percent deviations with lab data that fall within 5-10%, with many conditions below 5% deviation. The model has been validated with scores of electrolyte systems over hundreds of unique conditions. Yet, AEM is more than a scientific tool; it is a catalyst for global change. By enabling a shift away from fossil fuels, it accelerates the adoption of electric vehicles and the deployment of grid-scale battery systems. In essence, AEM not only advances battery research but also propels us toward a cleaner and more sustainable energy future, making energy storage more efficient and cost-effective on a global scale. AEM is the engine driving the clean energy revolution, empowering the global battery R&D community with an evolving set of tools that help to shape a brighter, greener

AEM generates numerous separate reports, covering issues and quantities such as:

- **Transport Properties** (viscosity, conductivity, diffusivity, transference numbers, ionic hopping)
- **Thermodynamic Properties** (activity coefficients, osmotic coefficient, osmotic pressure, etc.)
- **Ion Association Speciation** (ion pairs, triple ions, solid solvates)
- **Solvent-to-ion Binding Energies and Solvation Numbers** for both cations and anions
- **Ligand-wise and Net Lithium Desolvation Energy and Kinetics**
- **Solvent and Solution Permittivity** and related **Dielectric Depression**
- **Transport Analysis of Double-Layer Regions** and related electrolyte properties therein
- **Attenuation of properties under Faradaic transport conditions**
- **Field Effects on solvent dipole orientation**, considering both ionic and surface charge fields
- **Arrhenius Analysis (Activation Energies)** of ten foremost electrolyte properties
- **Large-Scale Optimization of solvent composition**, given a multi-solvent system (there are about ten distinct optimization parameters that are considered).

## Commercial Impact

AEM's disruptive capability is unparalleled, redefining electrolyte modeling for contemporary systems. It uniquely captures the intricacies of electrolyte behavior in electrochemical cells, making it highly relevant for present and future electrolyte development. With no peer in its class, AEM is poised to significantly accelerate domestic battery development, aligning perfectly with our ambitious vehicle and energy goals in the 21st century. By providing an unprecedented level of insight into electrolyte systems, AEM empowers researchers to optimize battery technologies rapidly. This translates to enhanced battery performance, extended lifespans, and reduced costs, which are all essential factors for the widespread adoption of electric vehicles and the deployment of efficient grid-scale energy storage solutions. In addition to helping with the early determination of large expenditures, its small computing footprint has been packaged into an intuitive graphical user interface (GUI) through the joint goal and partnership of INL and Ridgetop to commercialize this innovative technology.

Moreover, AEM's capabilities have the potential to reduce our dependence on fossil fuels, thereby mitigating the impact of climate change. As we transition toward a more sustainable future, AEM plays a pivotal role by ushering in cleaner, more efficient energy solutions. On an aggregate, AEM's disruptive capabilities

extend far beyond the laboratory; they hold the promise of reshaping our energy landscape, fostering innovation, and accelerating the realization of a cleaner and more sustainable world.



## About Idaho National Laboratory (INL)

As one of 17 national labs in the U.S. Department of Energy complex, Idaho National Laboratory is home to more than 5,700 researchers and support staff focused on innovations in nuclear research, renewable energy systems, and security solutions that are changing the world. From discoveries in advanced nuclear energy to carbon-free energy options and to protecting our nation's most critical infrastructure assets, our talented team at INL is constantly pushing the limits to redefine what's possible. To find out more information about INL visit our website at [www.inl.gov](http://www.inl.gov).

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