



# **Software User Guide for the Advanced Electrolyte Model (AEM)**

## **Developed by Idaho National Laboratory (INL)**

**Prepared and Distributed by:**

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## Advanced Electrolyte Model (AEM)

### Revision Record

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1.0 May 31, 2023	First release.
1.1 June 07, 2023	Second release with notes for Trial Version.
1.2 February 05, 2024	Third release with new salts and solvents with AEM version 2.24.1.
1.3 July 12, 2024	Fourth release with AEM ACCC Module and AEM Python API.
1.4 Aug 23, 2024	Fifth release with updates and ACCC functionality for Python API.

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## Advanced Electrolyte Model (AEM)

1	Introduction to the Advanced Electrolyte Model (AEM) .....	1
1.1	Technology Introduction and Overview.....	2
1.2	Selected Key Features.....	5
1.3	Technology Summary.....	6
2	AEM Installation.....	7
2.1	System Requirements.....	7
2.2	Software Installation and License Activation.....	7
3	AEM Graphical User Interface (GUI).....	12
3.1	AEM GUI Overview .....	12
3.2	AEM Input Tab.....	12
3.2.1	SOLVENT COMPOSITION .....	13
3.2.2	SELECT SOLVENTS.....	13
3.2.3	SELECT SALTS.....	19
3.2.4	TEMPERATURE SETTINGS.....	23
3.2.5	METHOD FOR HANDLING TRIPLE ION STABILITY .....	24
3.2.6	ELECTROLYTE INGRESS INTO PORES.....	24
3.2.7	SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP) .....	25
3.2.8	DOUBLE LAYER (DL).....	26
3.2.9	AEM RUN IDENTIFIER .....	27
3.2.10	RUN AEM .....	28
3.3	AEM Arbitrarily Chosen Chemical Compounds (ACCC) Module.....	31
3.3.1	AEM ACCC Solvent Class .....	32
3.3.2	Example of AEM ACCC Solvent Class.....	37
3.3.3	AEM ACCC Salt Class.....	38
3.3.4	Example of AEM ACCC Salt Class .....	41
3.3.5	Example of ACCC Validation .....	42
3.4	AEM Output Tab.....	44
3.4.1	AEM RUNS.....	45
3.4.2	AEM REPORTS.....	46
3.4.3	Data Display.....	47
3.4.4	REPORT TEXT.....	48

3.4.5	REPORT DATA VISUALIZATION.....	49
3.4.6	REPORT DATA EXTRACTION .....	50
3.5	Global Features & Icons .....	53
4	Examples.....	59
4.1	Example 1: Fixed Volume Proportions for 3-Solvent, 1-Salt System .....	59
4.1.1	Example 1: Importing Example 1 Parameters .....	59
4.1.2	Example 1: Overview of Simulation Input Conditions .....	60
4.1.3	Example 1: Data Output & Discussion.....	61
4.2	Example 2: Fixed Mass Proportions for 8-Solvent, 2-Salt System .....	65
4.2.1	Example 2: Importing Example 2 Parameters .....	65
4.2.2	Example 2: Overview of Simulation Input Conditions .....	66
4.2.3	Example 2: Data Output & Discussion.....	67
4.3	Example 3: 3-Solvent with Fixed Volume Proportions and .....	72
4.3.1	Example 3: Importing Example 3 Parameters .....	72
4.3.2	Example 3: Overview of Simulation Input Conditions .....	73
4.3.3	Example 3: Data Output & Discussion.....	74
4.4	Example 4: Water-based 2-Salt System with Fixed Molar Proportion .....	78
4.4.1	Example 4: Importing Example 4 Parameters .....	78
4.4.2	Example 4: Overview of Simulation Input Conditions .....	79
4.4.3	Example 4: Data Output & Discussion.....	80
4.5	Example 5: Matrix Optimization of Electrolyte Formulation with 4 Solvent, 2 Salt System 84	
4.5.1	Example 5: Importing Example 5 Parameters .....	84
4.5.2	Example 5: Overview of Simulation Input Conditions .....	85
4.5.3	Example 5: Data Output & Discussion.....	86
4.6	Example 6: ACCC Simulation with one ACCC Salt Definition .....	87
4.6.1	Example 6: Importing Example 6 Parameters .....	88
4.6.2	Example 6: Overview of Simulation Input Conditions .....	89
4.6.3	Example 6: Data Output & Discussion.....	89
4.7	Example 7: Two Salt Simulation with one Default Library Salt and one ACCC Salt .....	94
4.7.1	Example 7: Importing Example 7 Parameters .....	94

## Advanced Electrolyte Model (AEM)

4.7.2	Example 7: Overview of Simulation Input Conditions .....	95
4.7.3	Example 7: Data Output & Discussion.....	96
5	AEM Command Line Interface (CLI) .....	100
5.1	AEM CLI Overview.....	100
5.2	AEM CLI Program Flow Chart.....	100
5.3	Running Example 1 with AEM CLI.....	101
5.3.1	Setup to Run Example 1 with AEM CLI.....	101
5.3.2	Section A: Input Electrolyte Component List and Proportions:.....	103
5.3.3	Section B: Input Other Simulation Conditions:.....	107
5.3.4	Section C: Choose whether Surface-Charge Attenuated Electrolyte Permittivity (SCAEP) Calculations are Performed:.....	109
5.3.5	Section D: Choose whether Double Layer (DL) Calculations are Performed:.....	110
5.3.6	Section E: Output Files.....	110
6	AEM Python API.....	113
6.1	API Architecture.....	113
6.2	Requirements and Dependencies.....	114
6.3	Installation and Execution.....	115
6.4	AEM API Usage .....	121
6.4.1	AEM Home Path and Program Name Setup.....	121
6.4.2	Define Electrolyte Compositions .....	121
6.4.3	Define Input Parameters .....	122
6.4.4	Initialize and Run the AEM API.....	122
7	Appendix .....	125
7.1	AEM Data Output Summary .....	125
7.1.1	Summary Table of AEM Outputs .....	125
7.1.2	Data Output Reports and Definition of Terms .....	131
7.2	AEM ACCC Solvent Class Examples.....	139
7.3	AEM ACCC Salt Class Examples .....	155
7.4	ACCC Validation Examples .....	159
7.5	List of Relevant Publications .....	166
7.6	Table of Figures .....	168

# **1 Introduction to the Advanced Electrolyte Model (AEM)**

## **Software License Agreement Background:**

BATTELLE ENERGY ALLIANCE, LLC (BEA), having its principal place of business at 2525 N. Fremont Avenue, Idaho Falls, ID 83415, is the management and operating contractor of the Idaho National Laboratory (INL) under the United States Department of Energy (DOE) Contract No. DE-AC07-05ID14517. BEA has granted RIDGETOP GROUP INC. exclusive distribution rights to make and distribute copies of the commercial product version of the Advanced Electrolyte Model (AEM) comprising of a jointly developed Graphical User Interface (GUI), AEM OBJECT CODE, and engineering services to support customer training and understanding of AEM data output.

Prior to software use and operation please review all terms and conditions covered in the standard AEM Software License Agreement (SLA).

## **About Idaho National Laboratory:**

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).

## **About Ridgetop Group:**

Ridgetop Group Inc., founded in 2000, is an established engineering and technology company that provides condition-based maintenance (CBM), prognostic health management (PHM), and reliability engineering solutions to government and commercial organizations around the world. Ridgetop and INL have formed a strong technology and business collaboration partnership that complements Ridgetop's background and reputation of providing customers with innovative products and solutions for aerospace, defense, transportation, energy, and industrial applications. Ridgetop is headquartered in Tucson, Arizona and has a dedicated staff of highly qualified researchers, engineers, and data scientists who support the business development team to design, develop, and deploy the most innovative solutions. Ridgetop is also an AS9100D and ISO9001:2015 certified organization by the Management Certification of North America (MCNA). More information on Ridgetop's complete list of products and services can be reviewed on the company website at [www.ridgetopgroup.com](http://www.ridgetopgroup.com).

## 1.1 Technology Introduction and Overview

Welcome, and congratulations on your purchase of the Advanced Electrolyte Model (AEM)! This innovative technology is a scientific modeling tool capable of exploring activity at the molecular level to simulate, diagnose, and predict electrolyte behaviors.

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 multi-component 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.

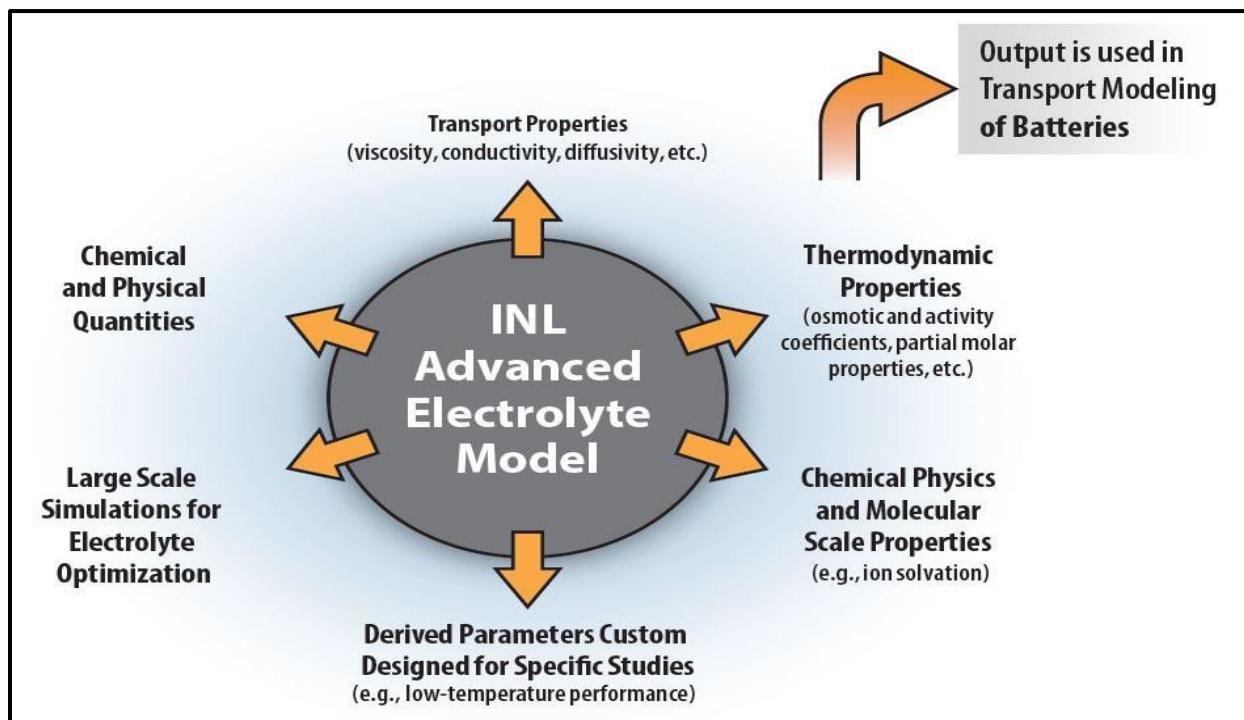


Figure 1. AEM Framework

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.

AEM is a proven capability designed to explore molecular-to-macroscale level aspects of electrolyte behavior and can be used to drastically reduce the time required to characterize and optimize electrolytes. Although it is applied most frequently to Li-ion and Na-ion battery systems, it is general in its theory and can be used toward numerous other targets.

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 the 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.

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.

More than just a tool to find a superior battery, 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 metabolic functions. This disruptive capability is unique, powerful, relevant to present and future electrolyte development, and without peer. It redefines electrolyte modeling for highly complex contemporary systems, wherein significant steps have been taken to capture the reality of electrolyte behavior in the electrochemical cell environment. This capability can have a very positive impact on accelerating domestic battery development to support aggressive vehicle and energy goals in the 21<sup>st</sup> century.

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

**Figure 2. 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).**

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

1. Transport Properties (viscosity, conductivity, diffusivity, transference numbers, ionic hopping)
2. Thermodynamic Properties (activity coefficients, osmotic coefficient, osmotic pressure, etc.)
3. Ion Association Speciation (ion pairs, triple ions, solid solvates)
4. Solvent-to-ion Binding Energies and solvation numbers for both cations and anions
5. Ligand-wise and net Lithium Desolvation energy and kinetics
6. Relative molal enthalpy
7. Solvent and Solution Permittivity, and related Dielectric Depression
8. Transport Analysis of Double-Layer Regions and related electrolyte properties therein
9. Attenuation of properties under Faradaic transport conditions
10. Field Effects on solvent dipole orientation, considering both Ionic and surface charge fields
11. Arrhenius Analysis (activation energies) of ten foremost electrolyte properties
12. Large-Scale Optimization of solvent composition, given a multi-solvent system (there are about ten distinct optimization parameters that are considered)
13. Summary of non-convergent cases
14. Many Other quantities

[Section 3.4.2](#) and [Section 7.1](#) provide more discussion of the output quantities generated by AEM.

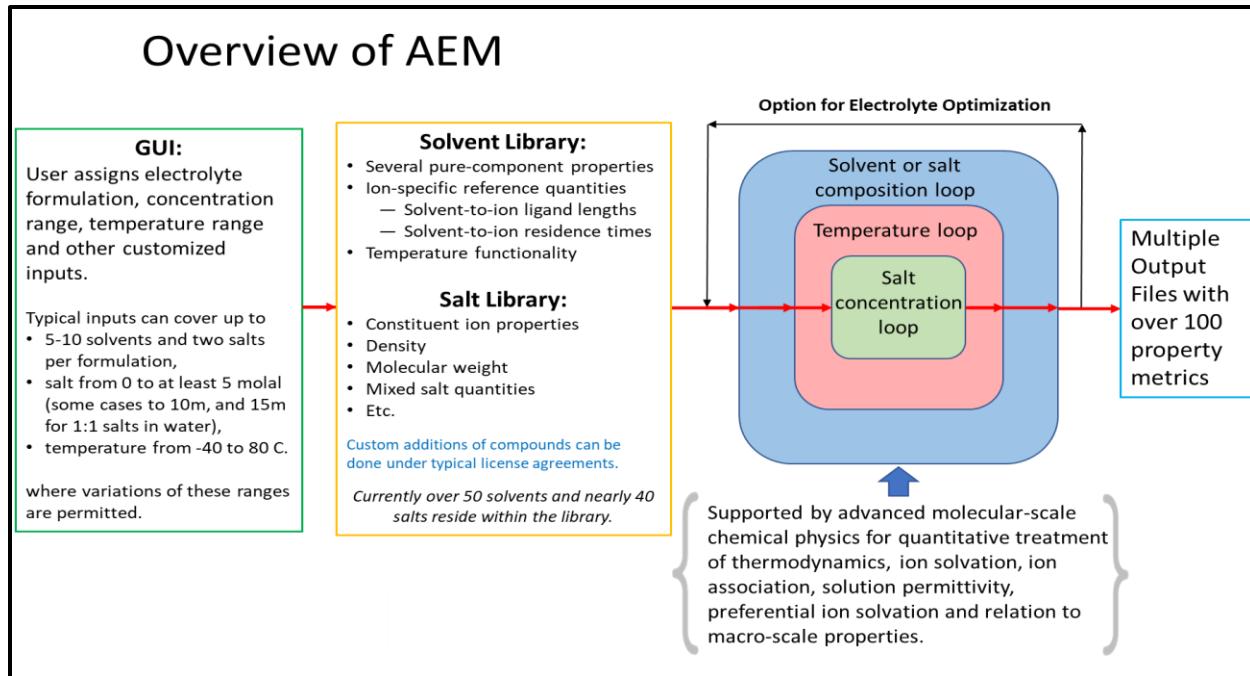


Figure 3. AEM Overview

## 1.2 Selected Key Features

- The chemical physics or statistical-mechanical basis of the AEM is found in the non-primitive non-restricted associative form of the Mean Spherical Approximation (NPNRAMSA), a powerful computational approach to accurate interpretation of chemical physics behind real electrolyte systems. The NPNRAMSA enables robust predictions over solvent composition, salt concentration, temperature, and permittivity domains.
- Added to this is an ion-solvation equation of state (IS-EOS) that renders accurate values of various quantities tied to ion solvation in such systems, such as effective solvated ion sizes, solvent-ion binding energies, solvation numbers, etc. The effects of ion solvation are central to the accurate prediction of all properties of electrolytes and cation (e.g., lithium) solvation/desolvation parameters.
- To address relevant contemporary electrolytes, the AEM accurately predicts the properties of multiple-solvent systems (up to 5 solvents or more) and handles two-salt systems.
- Key interfacial issues are targeted, including double-layer behavior, field effects on the solvent in the presence of the SEI, and lithium desolvation.
- The double-layer regions can and should exhibit local regions of non-electroneutrality, and hence, the AEM was developed to predict properties for such conditions.
- Contributing theories and mathematics are seamlessly integrated and self-consistent.
- AEM Component Database covers many battery-relevant solvents and salts and is growing.
- 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.

- The AEM has been used to help a growing list of private sector companies and DOE partners with electrolyte characterization and optimization, with more collaborations under development.

## **1.3 Technology Summary**

### **WHAT IS AEM?**

The Advanced Electrolyte Model (AEM) is a molecular-based computer simulation program created by Dr. Kevin Gering, a Distinguished Staff Scientist at Idaho National Laboratory, and is exclusively distributed by Ridgetop Group. It offers comprehensive and accurate theoretical relationships for the properties of complex electrolyte formulations and their influence on battery performance. Battery researchers use AEM to optimize electrolyte chemistries quickly and reduce energy storage costs worldwide. By lowering the cost of batteries, global dependence on fossil fuels can be diminished, and electric vehicle adoption and grid-scale battery system deployment can be accelerated. AEM can determine over 100 property metrics with each run, making it a virtual laboratory for genome-level electrolyte properties. It offers millions of combinations of over 60 solvents (and growing) and over 30 salts, allowing users to match their needs with a plausible set of candidates while balancing consequences for different choices of electrolytes. Over 20 reports are generated with each AEM run, covering properties that span transport, thermodynamic, physical, thermophysical, kinetic, molecular, and macroscale metrics.

### **Benefits**

- Accelerates battery development by quickly screening a wide array of materials for key properties, leading to time-to-market advantages.
- Provides a significant cost advantage compared to expensive empirical data collection techniques, reducing laboratory expenses for labor, analysis, and material requisition and disposal.
- Saves users significant time and resources, potentially translating to hundreds of thousands or even millions of dollars.
- Explores and reports with certainty and clarity on molecular-to-macroscale level aspects of electrolyte behavior, removing the guesswork in electrolyte qualification for specific applications.

### **Applications:**

- Battery manufacturers
- Automotive manufacturers
- Battery research institutions
- Lithium-ion and sodium-ion battery developers
- Energy system companies (petroleum and gas refining)
- Water processing and desalination industries
- Medical research institutions studying electrolytic functions in human cells
- Crystallization process industries
- Ion exchange system manufacturers

## 2 AEM Installation

### 2.1 System Requirements

The following requirements must be met to ensure proper system operation for executing both the AEM Graphical User Interface (GUI) and the legacy AEM Command Line Interface (CLI) software programs:

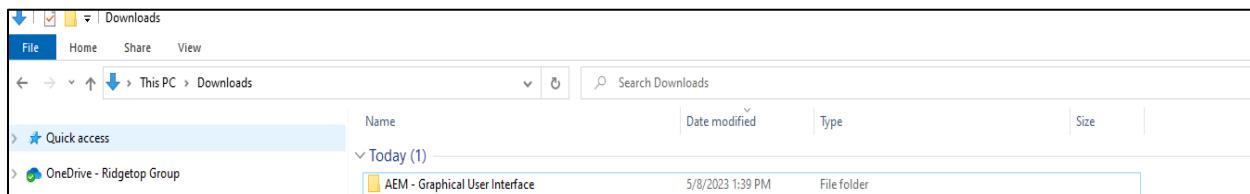
1. **Version:** AEM Version greater than or equal to **2.1.9 (released August 2024)**
2. **Compatibility:**
  - a. PC with **Windows 7 – Windows 11** operating system (**either 32 or 64-bit**). AEM is also adaptable to **MacOS** systems.
  - b. Laptop or Desktop architectures can be used. There is no need for a supercomputer or a special CPU/GPU design.
3. **Storage Requirements:**
  - a. Operating/executable files: **less than 500 MB**.
  - b. Report files generated during each run will vary in size depending on user inputs. In practical terms the total report file storage requirement is generally between **5 to 500 MB**.

**Important Note:** There is no specialized test equipment, hardware, or additional third-party software that needs to be purchased to run the AEM GUI. INL will provide initial guidance on software usage and oversee periodic updates to AEM during the license term. Ridgetop Group Inc. will facilitate AEM licensing, software distribution, and notification of updates. Updates can include additional compounds within the AEM library, new property sets, and overall improvements made to the GUI layout, output formatting and computing architecture.

### 2.2 Software Installation and License Activation

The AEM GUI can be installed by downloading the **AEM – Graphical User Interface** folder from an online filesharing system such as email, Dropbox, Box, or Ridgetop Group's website. Once downloaded, the following procedure can be followed to install and activate the software.

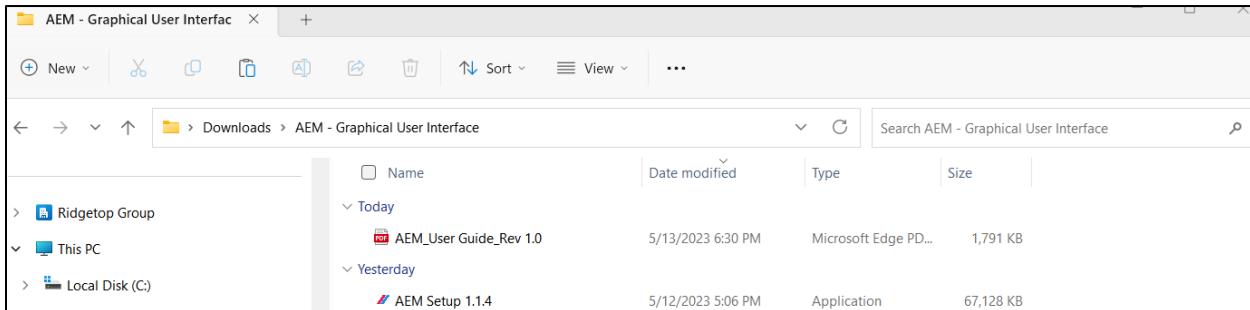
1. Download and extract the **AEM – Graphical User Interface** folder from the shared download source. Figure 4 provides a visual of this folder in Users default Downloads directory.



**Figure 4. AEM installation folder saved in This PC > Downloads.**

## Advanced Electrolyte Model (AEM)

2. Use the Windows File Explorer to open the **AEM – Graphical User Interface** folder and verify that the AEM User Guide and AEM Setup executable is inside the downloaded folder.

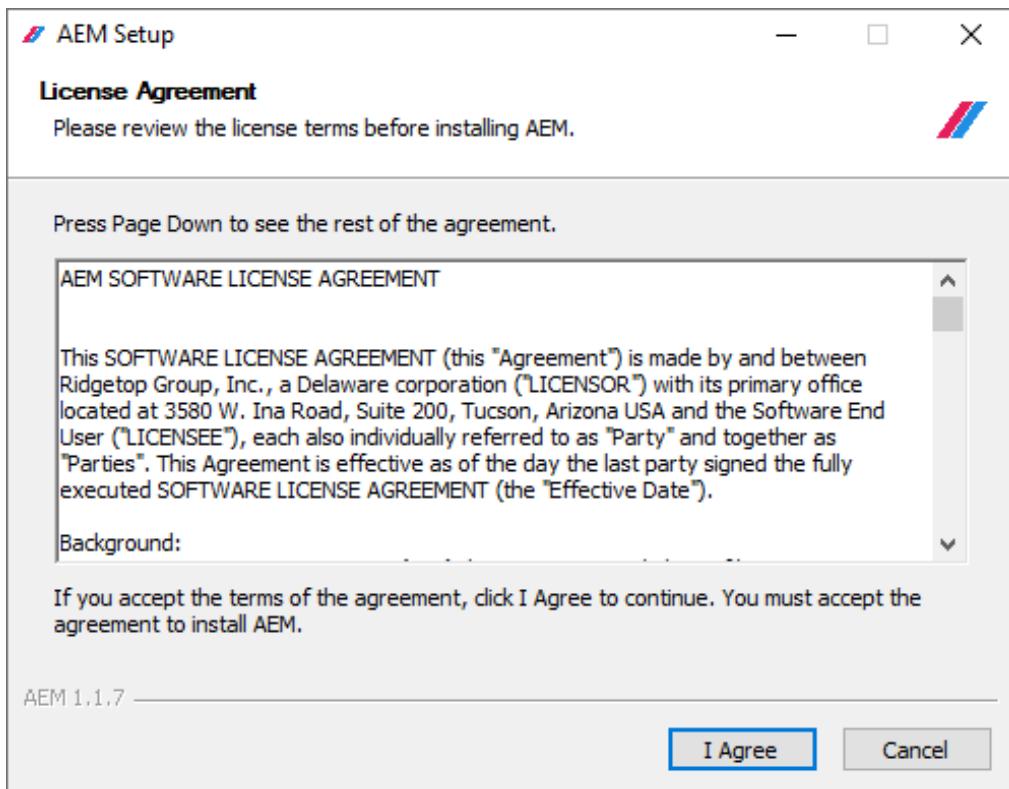


**Figure 5. The folder is located at This PC\Downloads\[AEM Download Path].**

3. Right-click on the **AEM Setup x.x.x.exe** or **AEM Trial Setup x.x.x.exe** and select **Run as Administrator**.

**Important Note:** **x.x.x** represents the AEM GUI version, and your version may be different if it was compiled during a later software release.

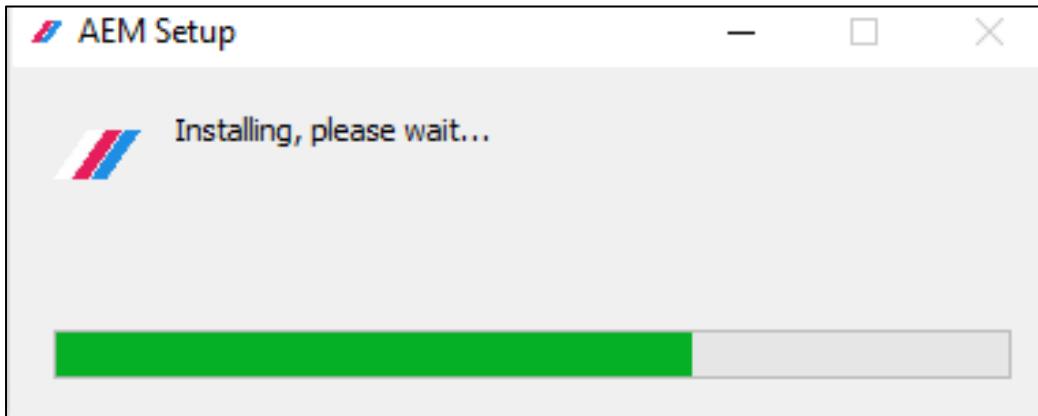
4. Verify that the installation wizard initializes as shown in Figure 6.



**Figure 6. AEM installation wizard initializing.**

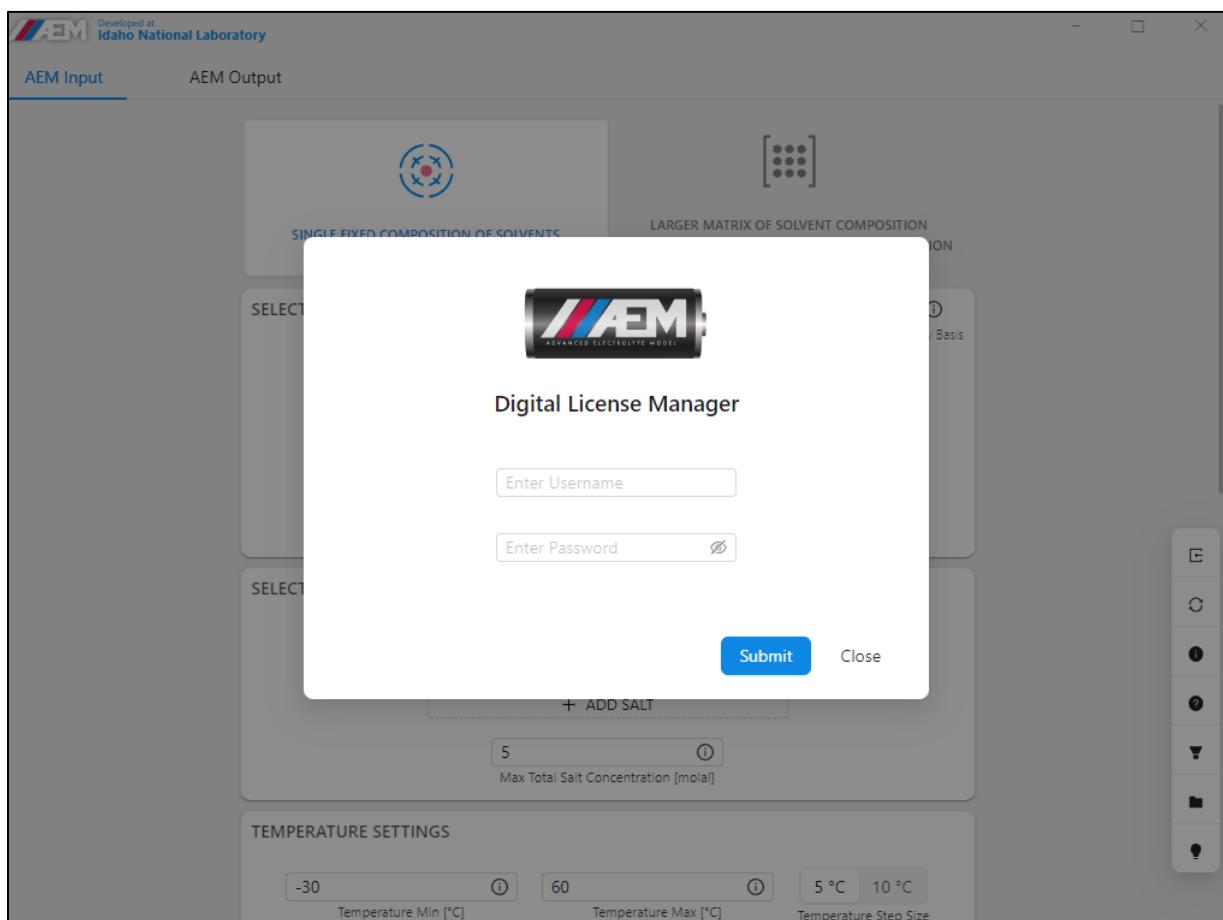
## Advanced Electrolyte Model (AEM)

- Accept the AEM Software License Agreement terms by clicking **I Agree** and wait for the installation wizard to complete as shown in Figure 7:



**Figure 7. View of the installation wizard for the AEM installation directory. Click Next>> to continue.**

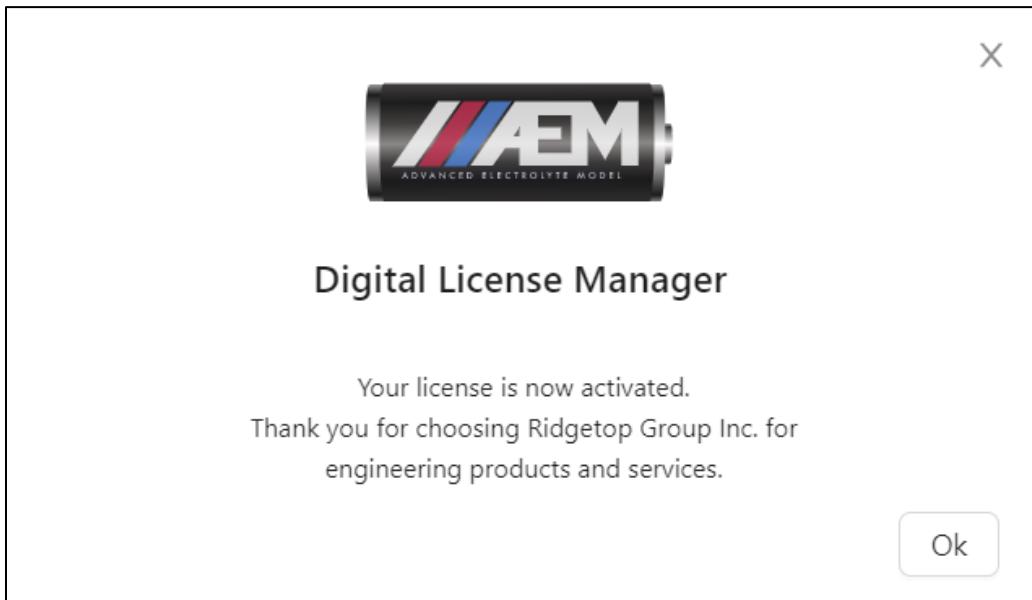
- Verify that AEM GUI starts as shown in Figure 8.



**Figure 8. View of the AEM GUI when it starts after a fresh installation.**

7. Enter your license username and password to activate your AEM software and verify that the pop-up message in Figure 9 appears.

**Important Note:** Each set of license credentials is linked to a unique computer ID for the term of the software license agreement (SLA) or the software trial period. Contact Ridgetop or INL directly if the license needs to be transferred to a new computer, or create a support ticket on the Ridgetop Group website: <https://www.ridgetopgroup.com/contact-us/support/>

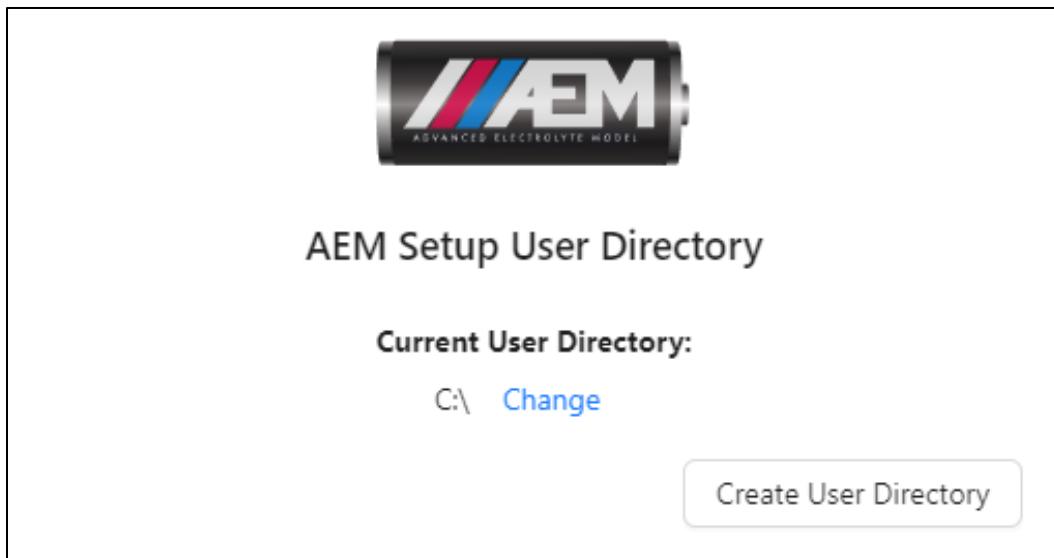


**Figure 9. AEM GUI pop-up indicating successful software license activation.**

8. After successfully activating your AEM software click **Ok** to continue and the AEM GUI shall prompt the user to specify their AEM User Directory as shown in Figure 10. The default program directory is outlined below:

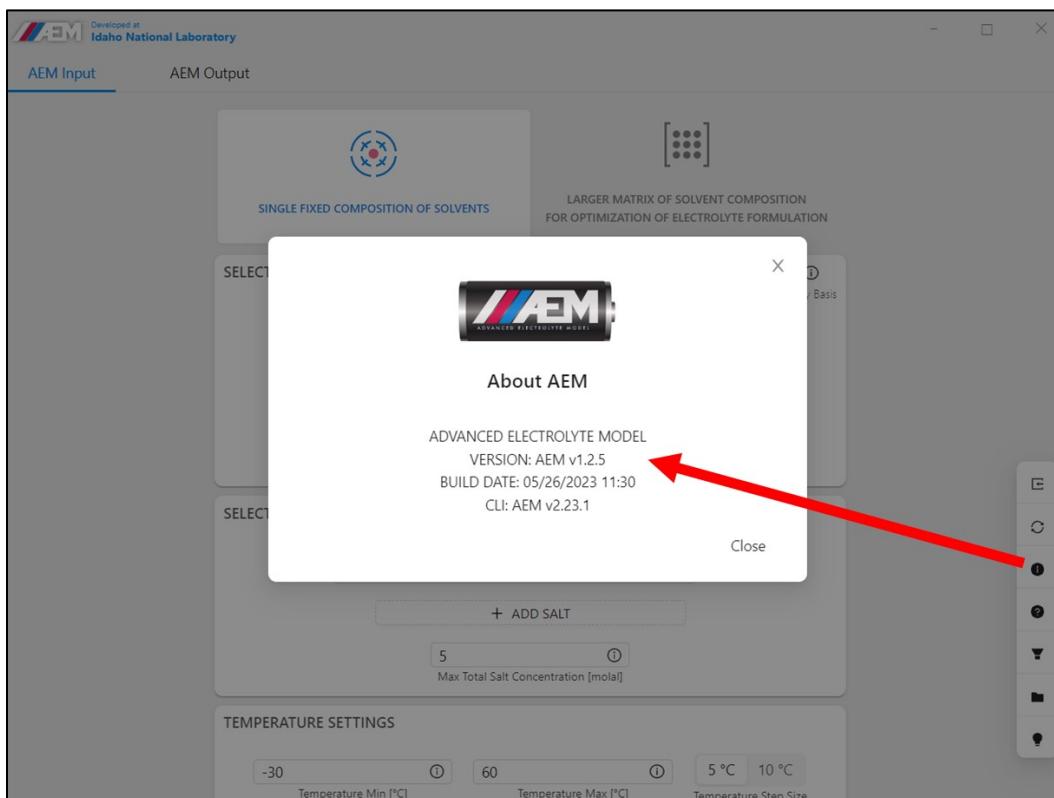
C:\Users\user-name\Documents\AEM\	Executable subdirectory
1. ACCC\	AEM ACCC Composition Files
2. CLI\	AEM Command Line Interface Directory
3. DATA\	AEM Data Output Files
3. EXAMPLES\	AEM Example Files

## Advanced Electrolyte Model (AEM)



**Figure 10. Selecting Default Program Directory during AEM Installation Process.**

9. Click the **About Icon** as shown in Figure 11 to verify that your AEM GUI installation is **greater than or equal to Version AEM V1.2.5** and that your AEM CLI Version is **greater than or equal to v2.23.1**.



**Figure 11. Verifying AEM Software Version.**

## 3 AEM Graphical User Interface (GUI)

This User Guide provides details regarding the AEM Graphical User Interface (GUI) software application, which is an extended product offering from the traditional AEM Command-Line Interface (CLI) program developed at Idaho National Laboratory (INL).

### 3.1 AEM GUI Overview

The AEM GUI is a Microsoft Windows-based Graphical User Interface (GUI) program that allows users to easily interact with the AEM CLI input conditions. The AEM GUI also allows users to save previous simulation runs and offers a built-in text previewing and plotting capability to analyze AEM data output reports and results.

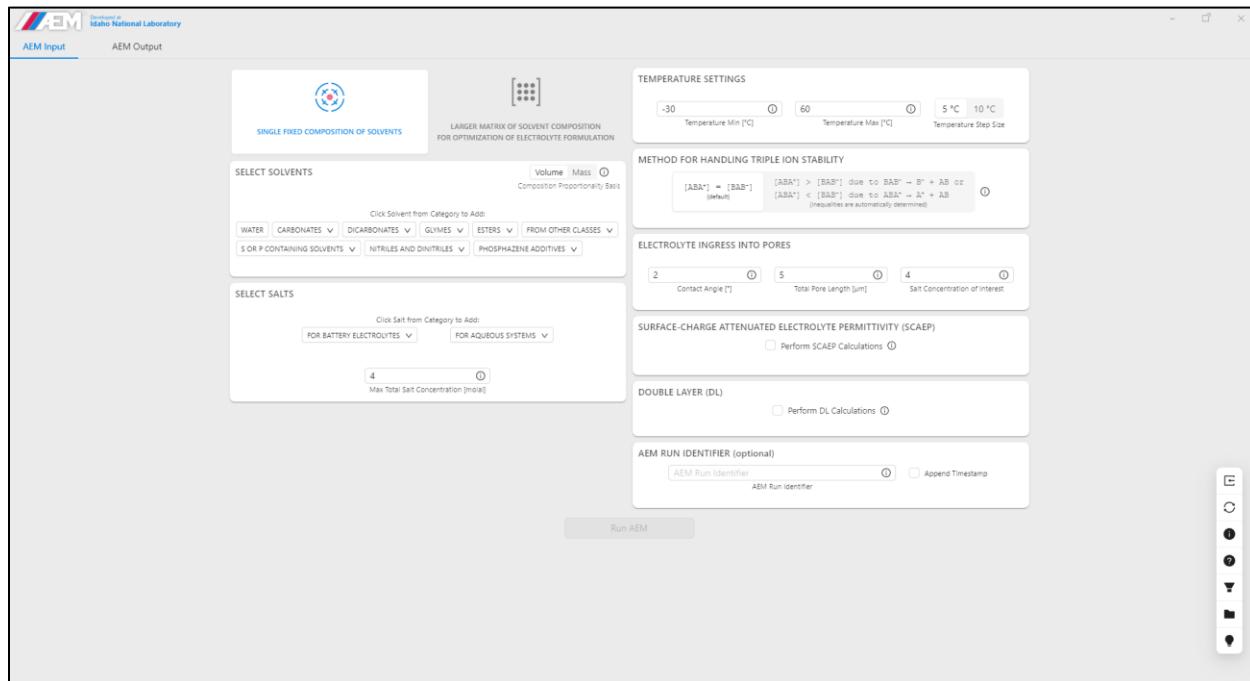
There are two main tabs in the AEM GUI as listed below:

1. AEM Input
2. AEM Output

Each tab offers a variety of checkboxes and parameters that a user can specify to run a simulation. The following sub-sections provide an overview of each tab.

### 3.2 AEM Input Tab

The AEM GUI has the following global simulation conditions as shown in Figure 12 on the first GUI tab.



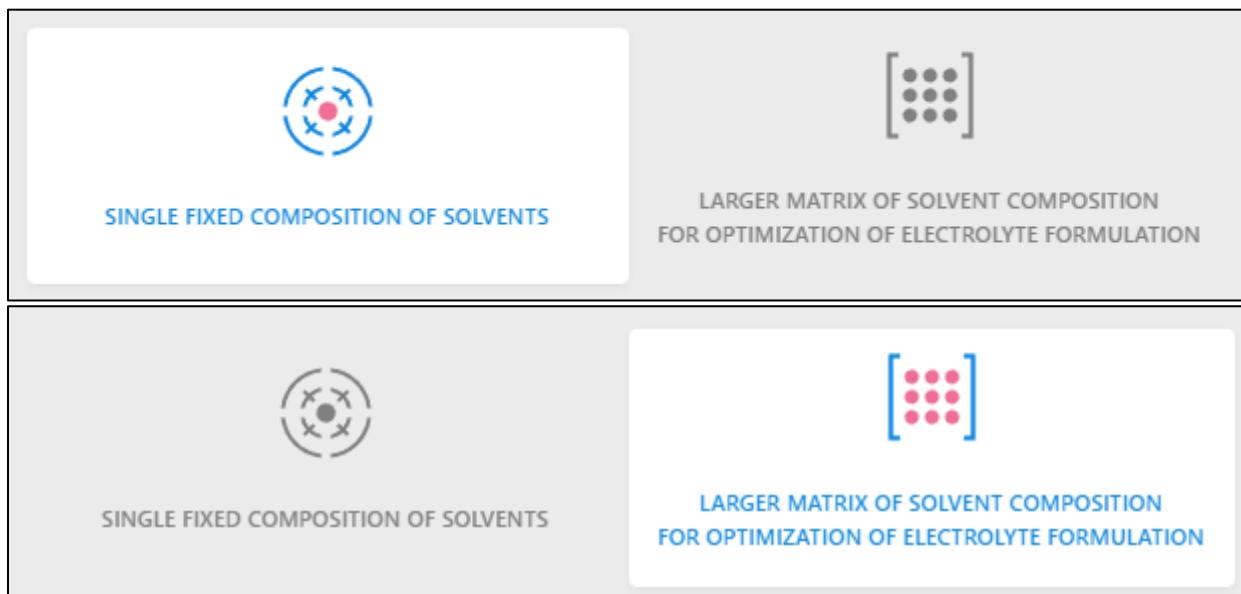
**Figure 12. Tab 1 – AEM Input.**

### 3.2.1 SOLVENT COMPOSITION

There are 2 available options for solvent composition to run an AEM simulation as listed below.

1. **SINGLE FIXED COMPOSITION OF SOLVENTS:** This will run a finite number of solvents to formulate the composition of the electrolyte.
2. **LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION:** This will run a matrix of solvents optimizing the process of formulating the electrolyte. This takes a longer time to run due to a larger time to process inputs.

The user can toggle between these options using the mode toggle switches shown in Figure 13 below. The option that is selected is displayed in a colored format with a box in the background.



**Figure 13. Solvent Composition Mode Toggle Switches in the AEM Input tab.**

### 3.2.2 SELECT SOLVENTS

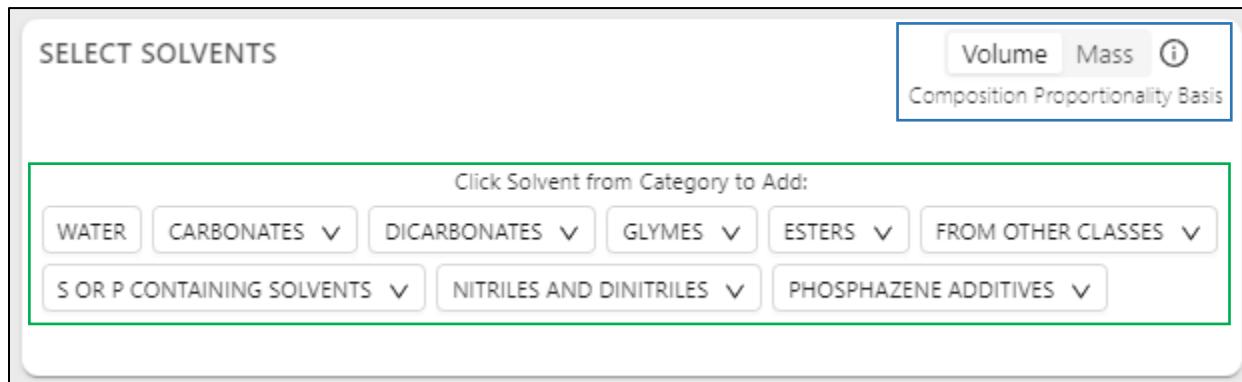
This is the section where the user defines the number and composition of solvents that are combined to formulate the desired electrolyte. The input to this section is highly dependent on what option the user decides to choose for the solvent composition as described in the previous section. Note that when the GUI is in the **Expanded Format**, the solvent selection list will be organized based on categories. When the GUI is in the **Compact Format**, the solvent selection list will be supported with a search capability to quickly type in the desired solvent name and/or abbreviation. Additional details on the **Expanded Format** vs. **Compact Format** are covered in [Section 3.5](#) where a visual aid was prepared in Figure 68.

#### FOR SINGLE FIXED COMPOSITION OF SOLVENTS:

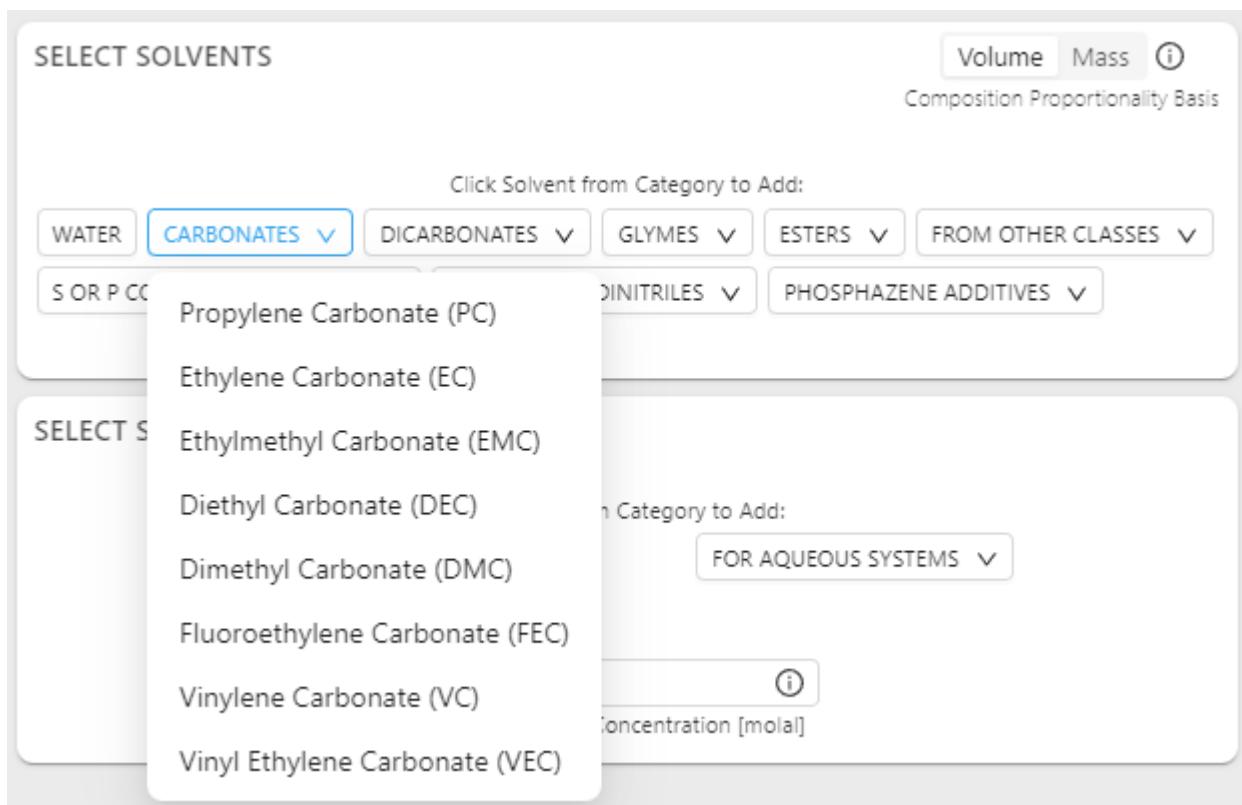
The maximum number of solvents allowed as inputs to the program in this option's case is **ten (10)**. The user can select the desired solvent using the drop-down list buttons classified according to the solvents' chemistries. The user also must supply an additional input by choosing the

## Advanced Electrolyte Model (AEM)

solvents' composition proportionality basis. This is achieved by using another toggle mode switch through which the user toggles between either **Volume** or **Mass**. A visual of this section with the drop-down list buttons (**green** box) and the mode toggle switch (**blue** box) is shown in Figure 14 below.



**Figure 14. SELECT SOLVENTS section for the SINGLE FIXED COMPOSITION OF SOLVENTS option of the AEM Input tab.**



**Figure 15. Drop-down List Button to select solvents for the SINGLE FIXED COMPOSITION OF SOLVENTS option of the AEM Input tab.**

Once the solvents have been defined and the composition proportionality has been set, there is one more input that the user must supply to the GUI. For each chosen solvent, the user must enter the percentage of the solvent by either **% Mass** or **% Volume** based on what was chosen for the

## Advanced Electrolyte Model (AEM)

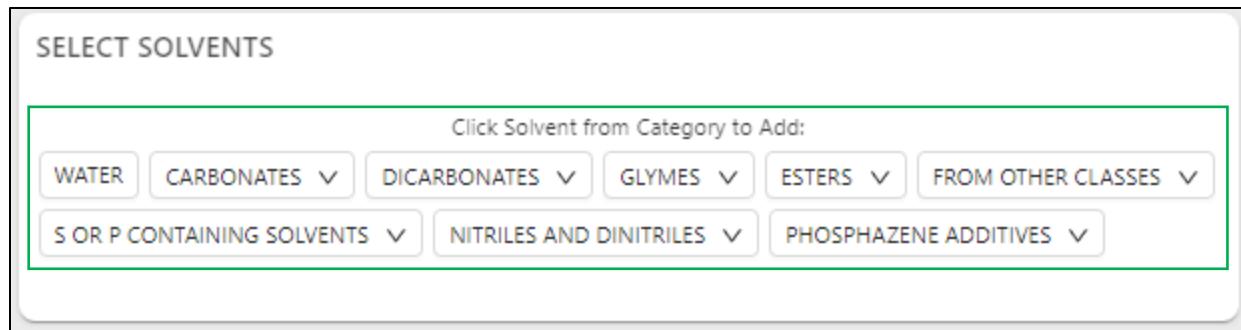
composition proportionality basis. This is shown in Figure 16 in which both the **Mass** and **Volume** cases are considered.

The figure consists of two vertically stacked screenshots of the "SELECT SOLVENTS" section of the AEM software. Both screenshots show a header with "SELECT SOLVENTS", "Volume", "Mass", and an information icon. Below this is a "Composition Proportionality Basis" section. Under "Click Solvent from Category to Add:", there are two rows of dropdown menus. The top row includes: WATER, CARBONATES, DICARBONATES, GLYMES, ESTERS, FROM OTHER CLASSES; S OR P CONTAINING SOLVENTS, NITRILES AND DINITRILES, PHOSPHAZENE ADDITIVES. The bottom row includes: CARBONATES / Propylene Carbonate (PC), ESTERS / Methyl Acetate (MA). Each entry has a "% Volume" or "% Mass" input field and a red minus sign button. The second screenshot is identical to the first but with the "Volume" tab selected instead of "Mass".

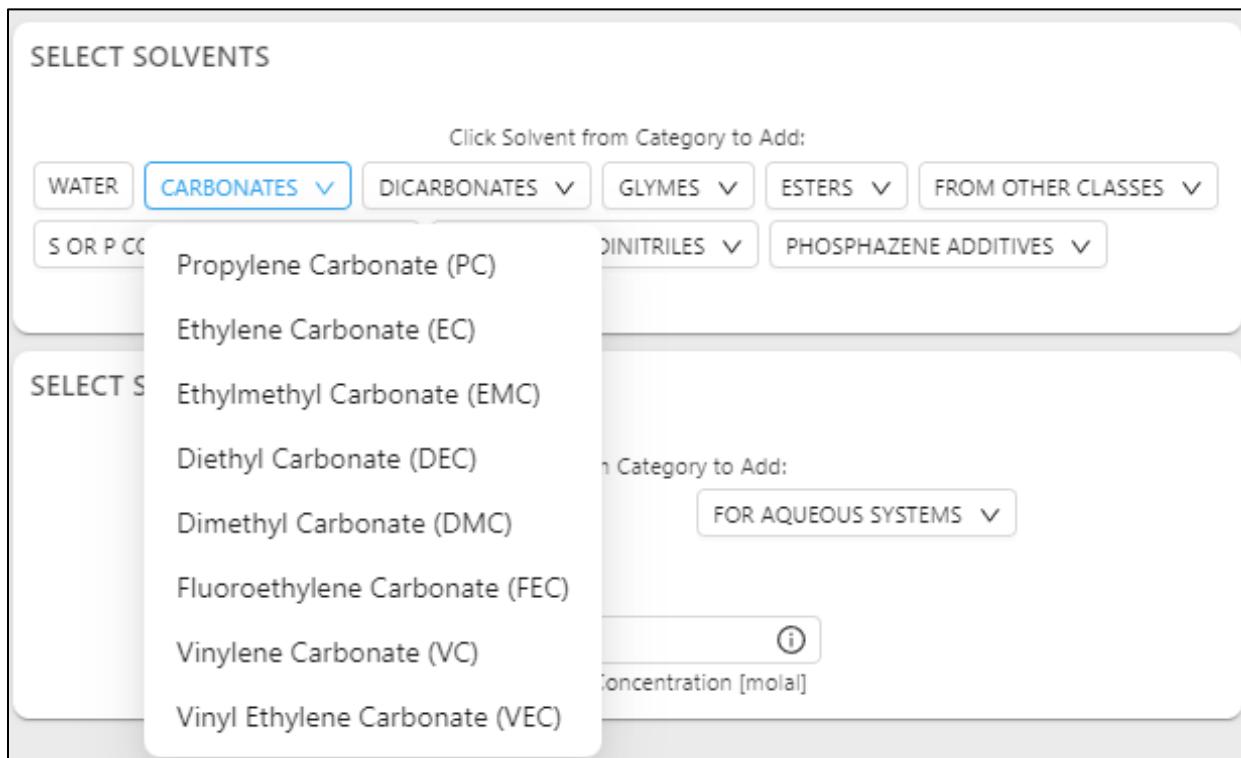
**Figure 16. Percentage of Solvent input depending on Volume/Mass for each solvent for the SINGLE FIXED COMPOSITION OF SOLVENTS option of the AEM Input tab.**

### FOR A LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION:

The maximum number of solvents allowed as inputs to the program in this option's case is **five (5)**. The user can select the desired solvent using the drop-down list buttons classified according to the solvents' chemistries. A visual of this section with the drop-down list buttons (**green** box) is shown in Figure 17 below.



**Figure 17. SELECT SOLVENTS section for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab.**



**Figure 18. Drop-down List Button to select solvents for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab.**

Once the solvents have been defined, there is no more input that the user must supply to the GUI, unless the user selects two (2) or more solvents. In that case, the user is given a choice to set the mass fraction of one (1) of the chosen solvents constant and define it between zero (0) and (1). For <=2 solvents, the visual of this section is shown in Figure 19. For <=2 solvents, the visual of this section is shown in Figure 20, where, for the solvent whose mass fraction is set constant, the user must define its value in the text box provided.

## Advanced Electrolyte Model (AEM)

**SELECT SOLVENTS**

Click Solvent from Category to Add:

**WATER** **CARBONATES** **DICARBONATES** **GLYMES** **ESTERS** **FROM OTHER CLASSES**

**S OR P CONTAINING SOLVENTS** **NITRILES AND DINITRILES** **PHOSPHAZENE ADDITIVES**

**ESTERS / Methyl Butyrate (MB)** **(-)**

**OTHER / 1NM2-Siloxane (1NM2)** **(-)**

This screenshot shows the 'SELECT SOLVENTS' section of the AEM Input tab. It displays a list of solvent categories and two specific solvents selected. The selected solvents are enclosed in green boxes with a minus sign icon to their right.

**Figure 19. SELECT SOLVENTS section for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab in the case of less than or equal to two (2) total solvents.**

**SELECT SOLVENTS**

Click Solvent from Category to Add:

**WATER** **CARBONATES** **DICARBONATES** **GLYMES** **ESTERS** **FROM OTHER CLASSES**

**S OR P CONTAINING SOLVENTS** **NITRILES AND DINITRILES** **PHOSPHAZENE ADDITIVES**

**ESTERS / Methyl Butyrate (MB)** **( Constant Mass Fracti**) **(-)**

**OTHER / 1NM2-Siloxane (1NM2)** **( Set Constant Mass Fraction**) **(-)**

**PHOSPHAZENE ADD. / INL Additive PA5** **( Set Constant Mass Fraction**) **(-)**

This screenshot shows the 'SELECT SOLVENTS' section of the AEM Input tab. It displays a list of solvent categories and three specific solvents selected. The first selected solvent has a checked checkbox next to it, indicating it is set to constant mass fraction. The other two selected solvents have unchecked checkboxes next to them, indicating they are not yet set to constant mass fraction.

**Figure 20. SELECT SOLVENTS section for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab in the case of greater than two (2) total solvents.**

AEM currently houses fifty-one (51) solvents of varying chemistries as shown in the list below. Ridgetop Group is currently working with INL to expand this list of available solvents.

## SOLVENTS

**1: water**

<b>CARBONATES</b>	<b>ESTERS</b>
2: propylene carbonate (PC)	9: ethyl acetate (EA)
3: ethylene carbonate (EC)	11: methyl butyrate (MB)
6: ethylmethyl carbonate (EMC)	12: ethyl propionate (EP)
7: diethyl carbonate (DEC)	13: n-propyl acetate (nPA)
8: dimethyl carbonate (DMC)	29: methyl acetate (MA)
15: fluoroethylene carbonate (FEC)	30: methyl propionate (MP)
39: vinylene carbonate (VC)	31: methyl formate (MF)
45: vinyl ethylene carbonate (VEC)	32: ethyl formate (EF)
	37: methyl monofluoroacetate (M1FA)
	38: methyl difluoroacetate (M2FA)
	58: ethyl difluoroacetate (E2FA)
	40: n-propyl propionate (nPP)
	42: n-butyl acetate (nBA)
	43: n-butyl propionate (nBP)
	44: n-butyl butyrate (nBB)
<b>DICARBONATES</b>	<b>NITRILES AND DINITRILES</b>
49: Dimethyl 2,5, Dioxahexanedioate (DMOHC)	26: glutaronitrile (GLN)
50: Diethyl 2,5, Dioxahexanedioate (DEOHC)	27: adiponitrile (ADN)
<b>GLYMES</b>	33: propionitrile (PrN)
5: 1,2 dimethoxyethane (DME)	36: acetonitrile (AN)
59: 1,2-dimethoxypropane (DMP)	41: butyronitrile (BN)
20: DEGDME (diglyme)	48: Succinonitrile (SN)
21: 3-TEGDME (triglyme)	61: isovaleronitrile (IVN)
22: 4-TEGDME (tetraglyme)	62: isobutyronitrile (IBN)
<b>S OR P CONTAINING SOLVENTS</b>	<b>FROM OTHER CLASSES</b>
16: ethylmethoxyethyl sulfone (EMES)	4: gamma-butyrolactone (GBL)
28: ethylmethyl sulfone (EMS)	10: 1,3 dioxolane
34: sulfolane (TMS)	14: ethylene glycol (EG)
35: trimethyl phosphate (TMP)	7: Dowanol-PMA (DOW-PMA)
55: triethyl phosphate (TEP)	18: 2-methoxyethyl acetate (MEA)
46: (proprietary, unavailable)	19: 1NM2-siloxane (1NM2)
60: dimethyl sulfite (DMS)	47: Tris(2,2,2-trifluoroethyl)-orthoformate (TFEO)
<b>PHOSPHAZENE ADDITIVES</b>	51: 7-oxabicyclo[2.2.1]heptane-2-carbonitrile (OCN)
23: Cyclic Phosphazene FM2	52: tetrahydrofuran (THF)
24: Cyclic Phosphazene SM4	53: (proprietary, unavailable)
25: Linear Phosphazene PA5	54: (proprietary, unavailable)
	56: Bis(2,2,2-trifluoroethyl) ether (BTFE)
	57: 1,1,1,1-trifluoroethyl-2.2.3.3-tetrafluoropropyl ether (TTE)

**Figure 21. Solvent list in AEM Version 2.24.1 with recent additions including 55-TEP, 56-BTFO, 57-TTE, 58-E2FA, 59-DMP, 60-DMS, 61-IVN, and 62-IBN. Note that only select solvents are available in the AEM Trial Version.**

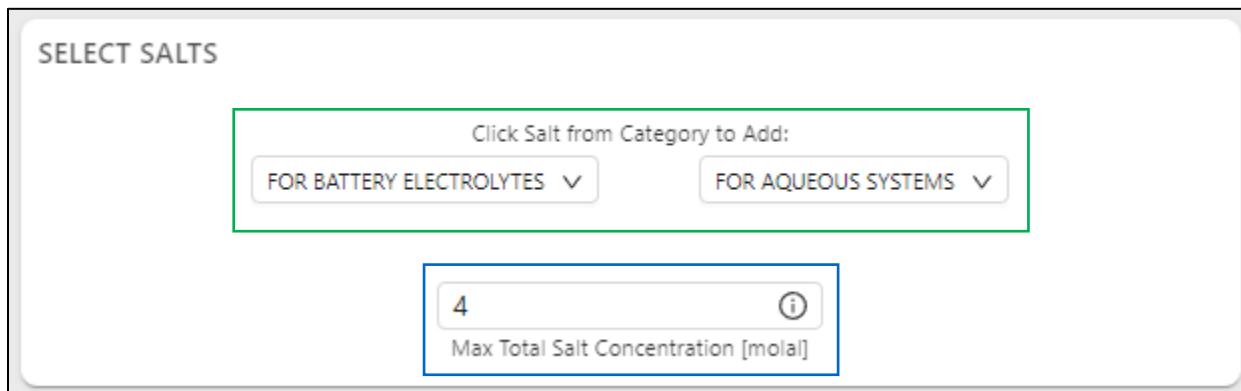
### 3.2.3 SELECT SALTS

This is the section where the user defines the number and composition of salts that are combined along with the chosen solvents to formulate the desired electrolyte. The input to this section is highly dependent on the number of salts chosen by the user – 1 or 2.

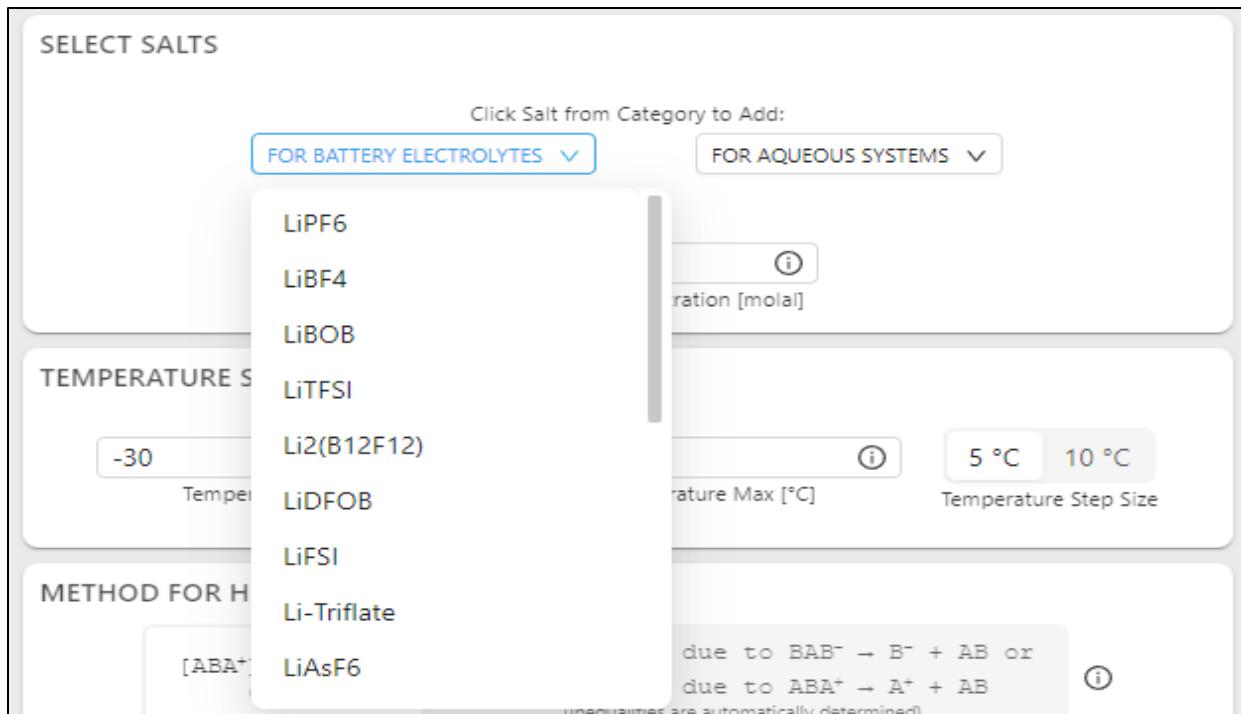
As previously mentioned with the solvent selection process, the **Expanded Format** and **Compact Format** will change how salts are selected for AEM simulation. When the GUI is in the **Expanded Format**, the salt selection list will be organized based on categories. When the GUI is in the **Compact Format**, the salt selection list will be supported with a search capability to quickly type in the desired salt name or abbreviation. Additional details on the **Expanded Format** vs. **Compact Format** are covered in [Section 3.5](#) where a visual aid was prepared in Figure 68.

**Important Note:** The maximum number of salts the user is allowed to choose is **two (2)**.

The user can select the desired salts using the drop-down list buttons classified according to the salts' chemistries – **FOR BATTERY ELECTROLYTES** and **FOR AQUEOUS SYSTEMS**. The user also must supply an additional text-box input by defining the maximum total salt concentration (**For battery electrolytes, this value falls between 6m to 8m, where m is molal units. This value can reach upwards of 15m when dealing with aqueous systems**). A visual of this section with the drop-down list buttons (green box) and the text box (blue box) is shown in Figure 22.



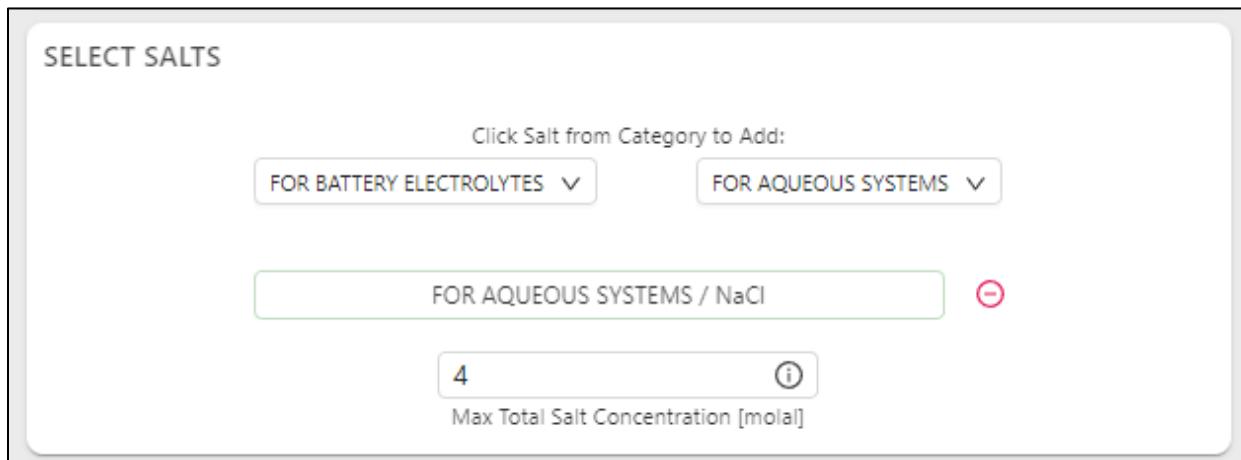
**Figure 22. SELECT SALTS section of the AEM Input tab.**



**Figure 23. Drop-down List Button to select salts for the SELECT SALTS section of the AEM Input tab.**

#### FOR ONE (1) SALT:

In the case that the user selects only one (1) salt, the only other input that must be supplied to the GUI is the maximum total salt concentration. This is shown in Figure 24, in which this case is considered with NaCl – common salt.

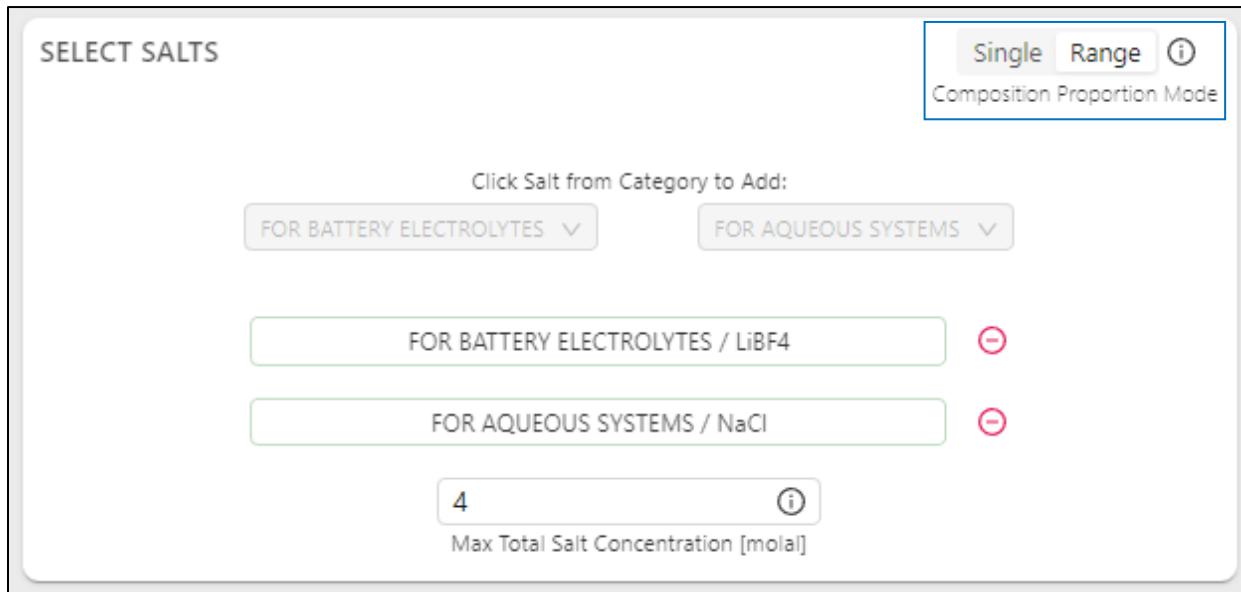


**Figure 24. SELECT SALTS section of the AEM Input tab for 1 salt.**

#### FOR TWO (2) SALTS:

In the case that the user selects two (2) salts, there is one other input that must be supplied to the GUI other than the maximum total salt concentration. The GUI provides a toggle mode switch

through which the user toggles between either **Single** or **Range** composition proportion mode for the salts. This is shown in Figure 25 in which this case is considered with LiBF<sub>4</sub> and NaCl – common salt with the toggle mode switch for the composition proportion mode (**blue** box).



**Figure 25. SELECT SALTS section of the AEM Input tab for 2 salts.**

**Single** mode will simulate **only one (1) mixed salt molar proportion**, while the **Range** mode will simulate **several proportions, covering mole fractions (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0)**. If the user selects the **Single** mode, the user must specify the percentage molar proportions or relative amount for each salt in the text boxes provided by the GUI. This is shown in Figure 26 in which this case is considered with LiBF<sub>4</sub> and NaCl – common salt with the text boxes for the molar percentages of the salts (**blue** box).

## Advanced Electrolyte Model (AEM)

SELECT SALTS

Single Range ⓘ  
Composition Proportion Mode

Click Salt from Category to Add:

FOR BATTERY ELECTROLYTES ▾ FOR AQUEOUS SYSTEMS ▾

FOR BATTERY ELECTROLYTES / LiBF4 % Molar ⚡

FOR AQUEOUS SYSTEMS / NaCl % Molar ⚡

4 ⓘ Max Total Salt Concentration [mola]

SELECT SALTS

Single Range ⓘ  
Composition Proportion Mode

Click Salt from Category to Add:

FOR BATTERY ELECTROLYTES ▾ FOR AQUEOUS SYSTEMS ▾

FOR BATTERY ELECTROLYTES / LiBF4 ⚡

FOR AQUEOUS SYSTEMS / NaCl ⚡

4 ⓘ Max Total Salt Concentration [mola]

**Figure 26. Single vs Range Composition Proportion Mode for the SELECT SALTS section of the AEM Input tab for 2 salts.**

AEM currently houses thirty-six (36) solvents of varying chemistries as shown in the list below. Ridgetop Group is currently working with INL to expand this list of available salts.

## SALTS

FOR BATTERY ELECTROLYTES	FOR AQUEOUS SYSTEMS
7: LiPF <sub>6</sub>	17: NaClO <sub>4</sub>
8: LiBF <sub>4</sub>	26: NaCl
9: LiBOB	27: NaNO <sub>3</sub>
10: LiTFSI	28: Na <sub>2</sub> SO <sub>4</sub>
11: Li <sub>2</sub> (B <sub>12</sub> F <sub>12</sub> )	29: LiNO <sub>3</sub>
12: LiDFOB	30: Li <sub>2</sub> SO <sub>4</sub>
38: <del>LiDFBOP</del>	31: MgSO <sub>4</sub>
13: LiFSI	32: Al(NO <sub>3</sub> ) <sub>3</sub>
14: Li-Triflate	33: LiBr
15: LiAsF <sub>6</sub>	34: NaOH
16: LiPO <sub>2</sub> F <sub>2</sub> (additive only)	35: KOH
17: NaClO <sub>4</sub>	36: LiOH
18: NaPF <sub>6</sub>	37: NaFSI
19: NaBF <sub>4</sub>	
20: NaTFSI	
37: NaFSI	
21: PA5-PF <sub>6</sub> (RTIL)	
22: PYR13-FSI (RTIL)	
23: EMI-FSI or EMIM-FSI (RTIL)	
24: CsPF <sub>6</sub>	
25: Mg(TFSI) <sub>2</sub>	

**Figure 27.** Salt list in AEM Version 2.24.1 with recent additions including 38-LiDFBOP.  
Note that only select Salts are available in the AEM Trial Version.

### 3.2.4 TEMPERATURE SETTINGS

This is the section where the user defines the temperature range along with the step size for that range in which the electrolyte will be used. The input from this section is essential for the calculation of properties over temperature to derive important thermodynamic quantities. The user can specify the **Temperature Min (°C)** and **Temperature Max (°C)** using text boxes provided by the GUI. The user must also supply an additional toggle mode switch input through which the user toggles between either **5°C** or **10°C** for the **Temperature Step Size**. A **5°C** step size **produces a finer grid and provides slightly better fidelity in Arrhenius calculations**. A **10°C** step size is recommended for the **LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION** option for **SOLVENT COMPOSITION** as it **reduces matrix by nearly half and provides coarser fidelity in Arrhenius calculations**. A visual of this section with the text boxes for the temperature inputs and the toggle mode switch for the temperature step size is shown in Figure 28.

**Important Note:** The temperature range allowed by AEM will cover all conditions for electrolyte systems under conventional use conditions. A typical range for non-aqueous electrolytes is **-30°C to 60°C** with lower and higher temperatures possible. It is recommended not to exceed 100 °C.

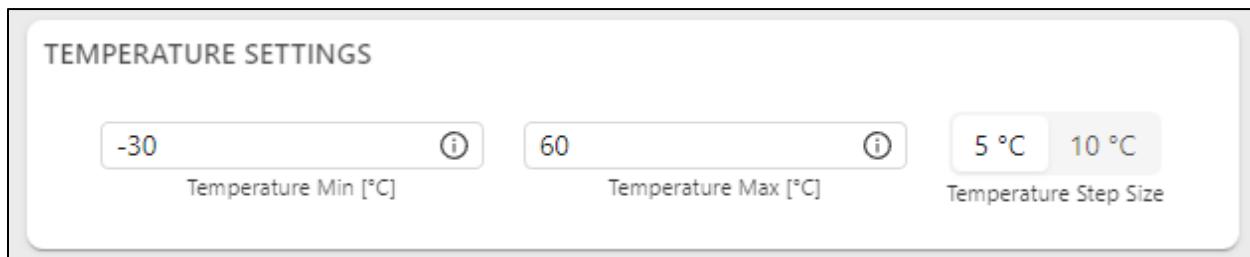


Figure 28. TEMPERATURE SETTINGS section of the AEM Input tab.

### 3.2.5 METHOD FOR HANDLING TRIPLE ION STABILITY

This is the section where the user defines the preferred approach for triple ion (TI) stability, whether the default is used ( $[ABA^+] = [BAB^-]$ ) or whether there is a subsequent conversion of either  $[ABA^+]$  or  $[BAB^-]$  into a single ion and an ion pair. The user must supply the preferred option using a toggle mode switch through which the user toggles between either  **$[ABA^+] = [BAB^-]$  (default)** or  **$[ABA^+] > [BAB^-]$  due to  $ABA^+ \rightarrow A^+ + AB$ , or  $[ABA^+] < [BAB^-]$  due to  $ABA^+ \rightarrow A^+ + AB$  (inequalities are automatically determined)**. If the  **$[ABA^+] = [BAB^-]$  (default)** option is selected, the concentrations of cationic triple ions  $[ABA^+]$  and anionic triple ions  $[BAB^-]$  are assumed to be equal so that their ratio  $[ABA^+]/[BAB^-]$  equals 1. Whereas, if the  **$[ABA^+] > [BAB^-]$  due to  $ABA^+ \rightarrow A^+ + AB$ , or  $[ABA^+] < [BAB^-]$  due to  $ABA^+ \rightarrow A^+ + AB$  (inequalities are automatically determined)** option is selected, the ratio of  $[ABA^+]/[BAB^-]$  is recalculated to determine if there is cationic TI dominance (ratio > 1) or anion TI dominance (ratio < 1). These distinctions within the TI population have an impact on some properties such as the cation transference number. A visual of this section with the toggle mode switch to select the triple ion stability method is shown in Figure 29.

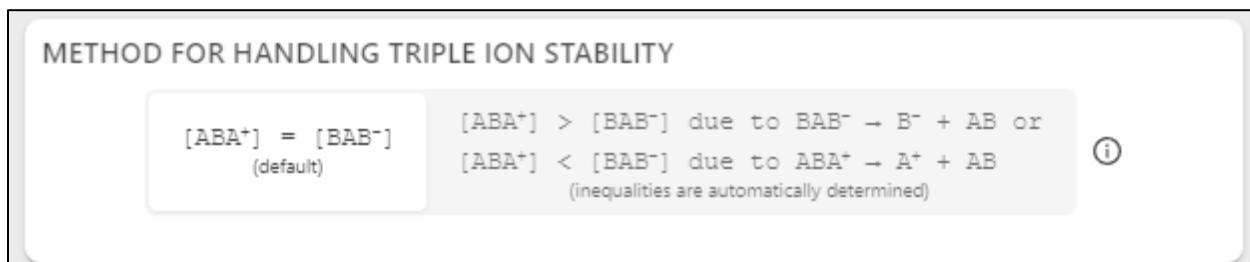


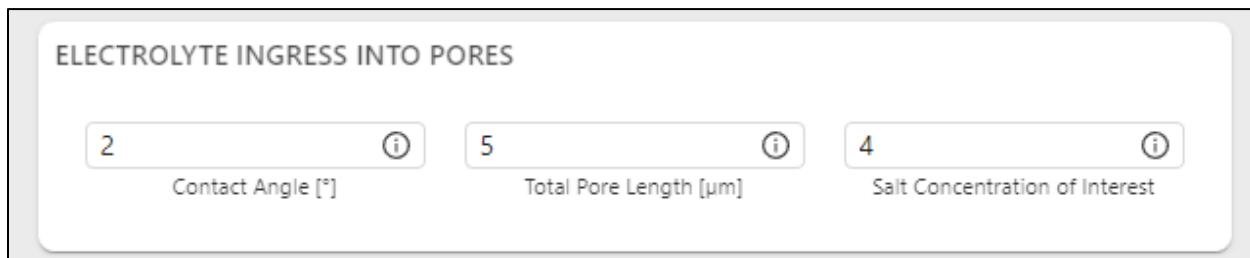
Figure 29. TEMPERATURE SETTINGS section of the AEM Input tab.

### 3.2.6 ELECTROLYTE INGRESS INTO PORES

This is the section where the user defines three inputs correlating to the permeation of the electrolyte in porous regions. The user can specify the **Contact Angle (°)**, **Total Length of Pore (μm)**, and **Salt Concentration of Interest (m)** using text boxes provided by the GUI. A visual of this section with the text boxes for the inputs described above is shown in Figure 28.

**Important Note:** The ranges allowed for the above inputs are as follows.

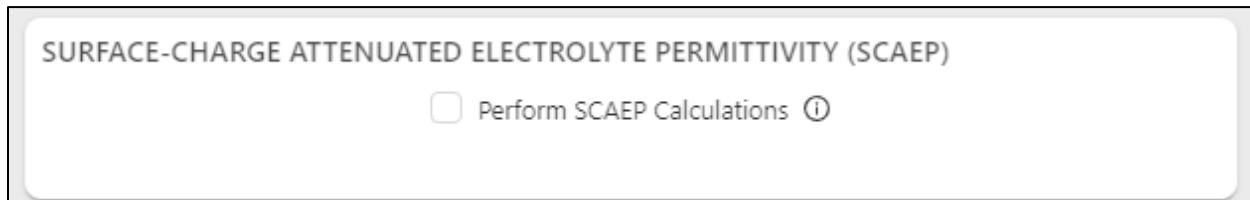
- **Contact Angle (°):** 0 – 90°
- **Total Length of Pore (μm):** 0.1 – 50μm
- **Salt Concentration of Interest (m):** Less than equal to (<=) the Maximum Salt Concentration, usually 0.1 – 8m



**Figure 30. ELECTROLYTE INGRESS INTO PORES section of the AEM Input tab.**

### 3.2.7 SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)

This is the section where the user defines certain inputs for the calculation of surface-charge effects on permittivity for electrolyte neighboring an electrode surface. Local electrolyte permittivity will be reduced by the presence of an electrode surface charge as would be present during actual battery operation. The GUI provides a **Perform SCAEP Calculations** check box that allows the user to turn the SCAEP calculations on and off. A visual of this section with the check box not checked (SCAEP calculations turned off) (default) is shown in Figure 31.



**Figure 31. SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP) section of the AEM Input tab with a check box to perform SCAEP Calculations not checked (default).**

If the check box is checked and the SCAEP calculations are turned on, the GUI prompts the user to specify some new inputs. Using a toggle mode switch, the user must specify the **Type of Pulse Condition** between either **Discharge** or **Charge**. Subsequently, the user can specify the **Cell Voltage of Interest (V)**, **Bulk Salt Concentration (molal)**, **Thickness of Cathode/Anode SEI (Å)**, **Relative Permittivity of Cathode/Anode SEI (%)**, and **Average Porosity of Cathode/Anode SEI (ε)** using text boxes provided by the GUI. A visual of this section with the toggle mode switch and text boxes for the inputs described above is shown in Figure 32.

**Important Note:** The ranges allowed for the above inputs are as follows.

- **Cell Voltage of Interest (V):** 3 – 4.5V [Specific to Li-ion Cells]
- **Bulk Salt Concentration (molal):** 0.2 – 3.8m
- **Thickness of Cathode/Anode SEI (Å):** 10 – 100Å, typically between 200 – 400Å
- **Relative Permittivity of Cathode/Anode SEI (%):** 2 – 100%, typically 10 – 20%

- **Average Porosity of Cathode/Anode SEI ( $\epsilon$ ):** 0.05 – 0.9, typically 0.2 – 0.4

The screenshot shows two identical sections of the AEM Input tab, each titled "SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)". Each section contains a checked checkbox labeled "Perform SCAEP Calculations". Below the checkbox are four input fields: "Type of Pulse Condition" (radio buttons for "Discharge" and "Charge"), "Cell Voltage of Interest [V]" (set to 3.5), "Bulk Salt Concentration [m]" (set to 3.5), and three numerical inputs with units: "Thickness of Cathode SEI [Å]" (200), "Rel. Permittivity of Cathode SEI [%]" (10), and "Ave. Porosity of Cathode SEI [ $\epsilon$ ?]" (0.2). The second section is identical, with "Type of Pulse Condition" set to "Charge", "Cell Voltage of Interest [V]" set to 3.5, "Bulk Salt Concentration [m]" set to 3.5, and numerical inputs for "Thickness of Anode SEI [Å]" (200), "Rel. Permittivity of Anode SEI [%]" (10), and "Ave. Porosity of Anode SEI [ $\epsilon$ ?]" (0.2).

**Figure 32. SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP) section of the AEM Input tab with a check box to perform SCAEP Calculations checked.**

### 3.2.8 DOUBLE LAYER (DL)

This is the section where the user specifies inputs to facilitate double-layer (DL) calculations. These calculations are done over a fine grid of spatial (1D, 5nm steps) and time dimensions, allowing the determination of electrolyte gradients and related properties in the anode and cathode double layers. These calculations are done over relatively short periods to reveal the emergent dynamic of the electrolyte gradients. The GUI provides a **Perform DL Calculations** check box that allows the user to turn the DL calculations on and off. A visual of this section with the check box not checked (DL calculations turned off) (default) is shown in Figure 31.

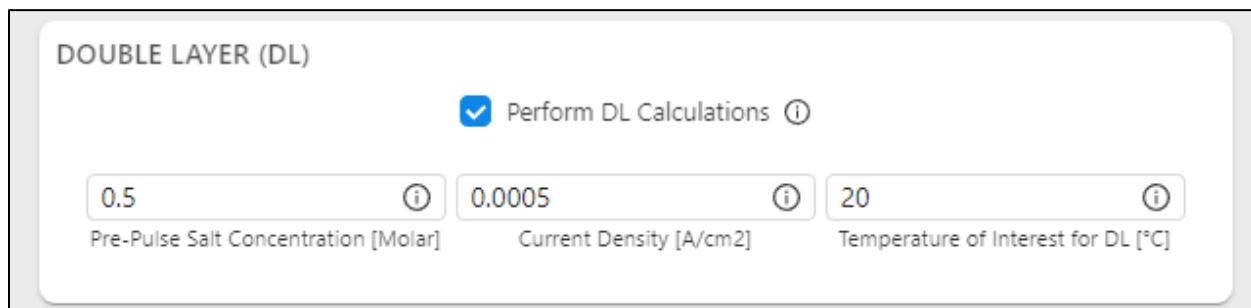
The screenshot shows the "DOUBLE LAYER (DL)" section of the AEM Input tab. It features a label "DOUBLE LAYER (DL)" and a checkbox labeled "Perform DL Calculations". The checkbox is currently unchecked, indicating that DL calculations are turned off by default.

**Figure 33. DOUBLE LAYER (DL) section of the AEM Input tab with check box to perform DL Calculations not checked (default).**

If the check box is checked and the DL calculations are turned on, the GUI prompts the user to specify some new inputs. The user can specify the **Pre-Pulse Salt Concentration (molar)**, **Current Density (A/cm<sup>2</sup>)**, and **Temperature of Interest for DL (°C)** using text boxes provided by the GUI. A visual of this section with the text boxes for the inputs described above is shown in Figure 34.

**Important Note:** The ranges allowed for the above inputs are as follows.

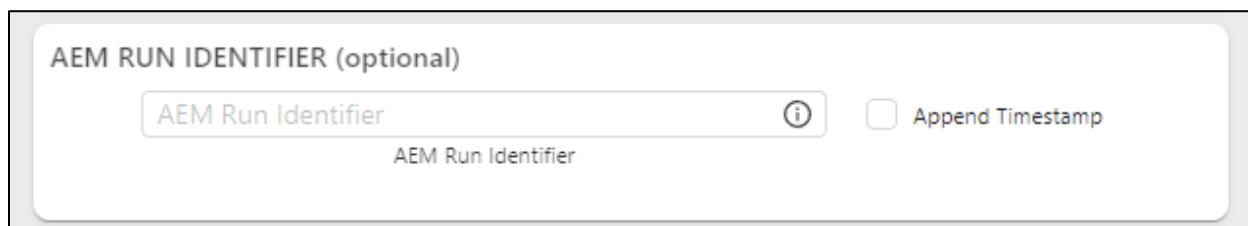
- **Pre-Pulse Salt Concentration (molar):** 0.5 – 1.5 molar
- **Current Density (A/cm<sup>2</sup>):** 0.00001 – 0.1 A/cm<sup>2</sup>
- **Temperature of Interest for DL (°C):** Between T<sub>min</sub> and T<sub>max</sub> defined in section 3.2.4. Should be at a decade of °C, for example, -10°C, 0°C, 10°C, and so on



**Figure 34. DOUBLE LAYER (DL) section of the AEM Input tab with a check box to perform DL Calculations checked.**

### 3.2.9 AEM RUN IDENTIFIER

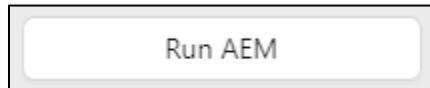
This is the section where the user can specify optional inputs to add a custom name to the AEM run and record the time when the AEM simulation was run. All the reports generated by AEM (as well as an import file) will be stored in **C:\Users\user-name\Documents\AEM\DATA\** after a run. When the **Append Timestamp** check box is selected, the folder will be saved with your **AEM Run Identifier** followed by a timestamp in the form of **AEM Run Identifier-YYYYMMDD\_hhmmss**, where **YYYYMMDD** is the format for **Date (i.e., YYYY-MM-DD)** and **hhmmss** is the format for **Time (i.e., hh:mm:ss)**. If the check box is not selected, then the folder will simply be named whatever is in the **AEM Run Identifier** text field. If the folder already exists for that run, the directory will append a number in parentheses depending on how many runs with the same name exist. A visual of this section is shown in Figure 35.



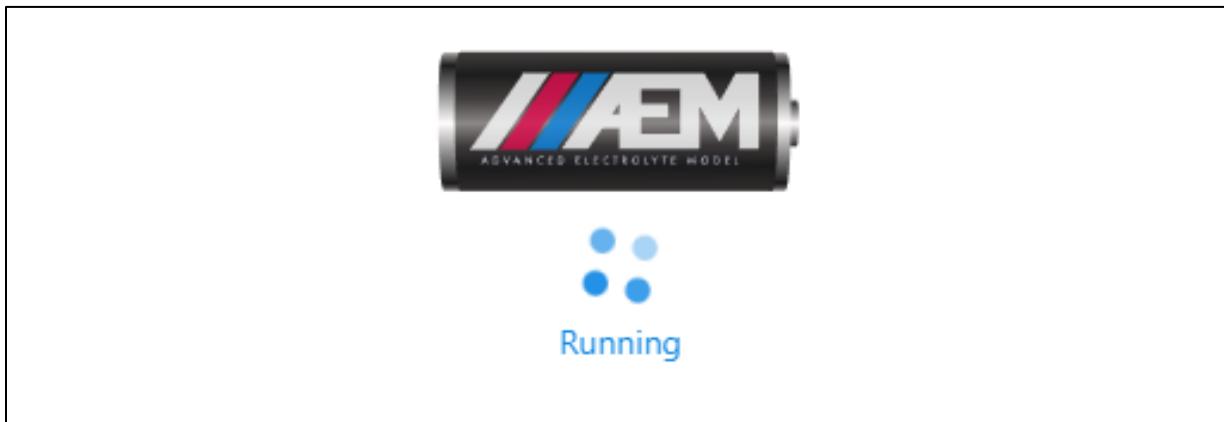
**Figure 35. AEM RUN IDENTIFIER section of the AEM Input tab.**

### **3.2.10 RUN AEM**

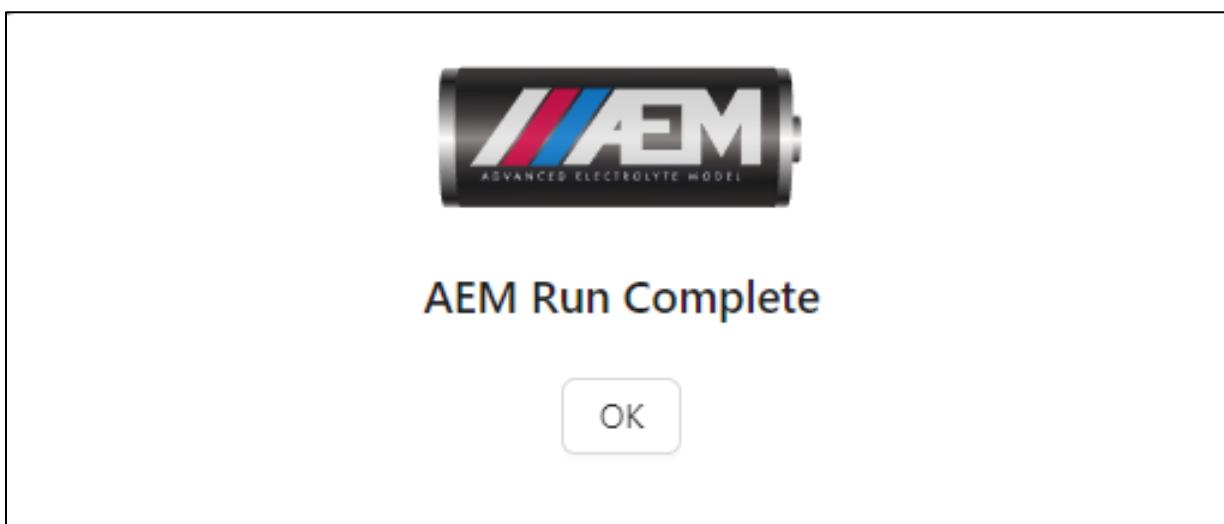
This is the last step after the input conditions for a particular AEM simulation have been entered or imported using the **Import** button described in section 3.5. The GUI provides a **Run AEM** as shown in Figure 36, which upon clicking initiates the start of the AEM simulation. Shown in Figure 37 is what happens after the button is clicked and Figure 38 is the prompt the GUI throws when the AEM simulation is complete.



**Figure 36. RUN AEM Button of the AEM Input tab.**



**Figure 37. Prompt showing AEM running after the RUN AEM Button of the AEM Input tab is clicked.**



**Figure 38. Prompt showing AEM Run Complete.**

## Advanced Electrolyte Model (AEM)

In the case that the AEM simulation fails, the GUI will prompt an error message as shown in Figure 39 and record a **ERROR\_OCCURRED.txt** text file in the directory for the current simulation in **C:\Users\user-name\Documents\AEM\DATA\**. A visual of where this file is located and how it looks in a text editor is shown in Figure 40 and Figure 41, respectively.

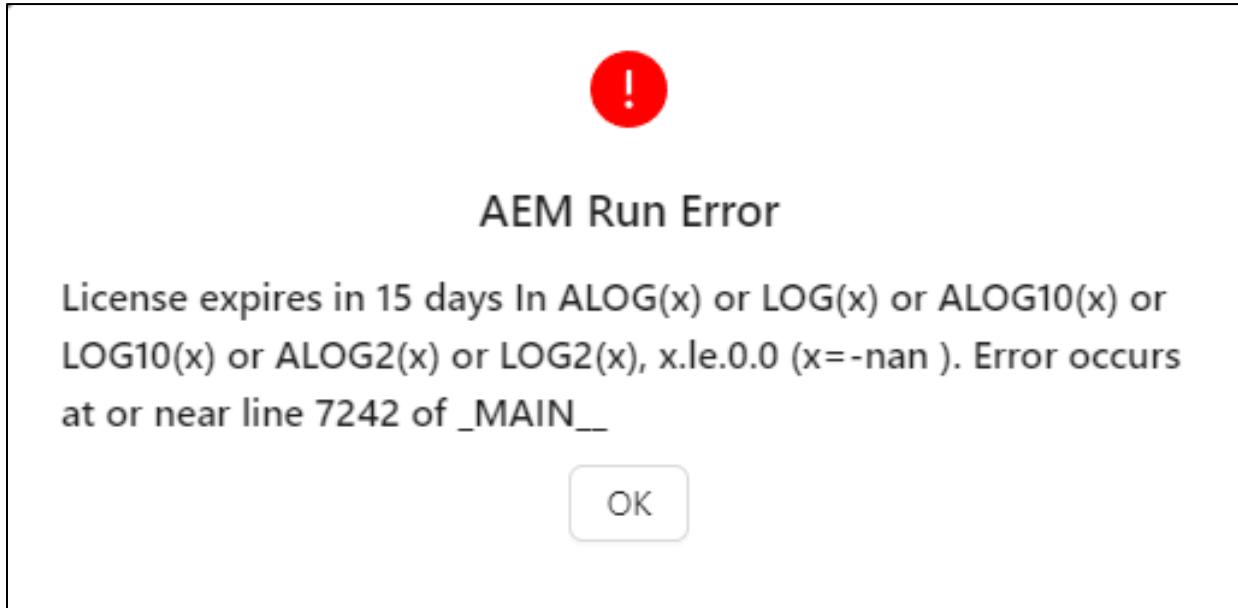


Figure 39. AEM Run Error.

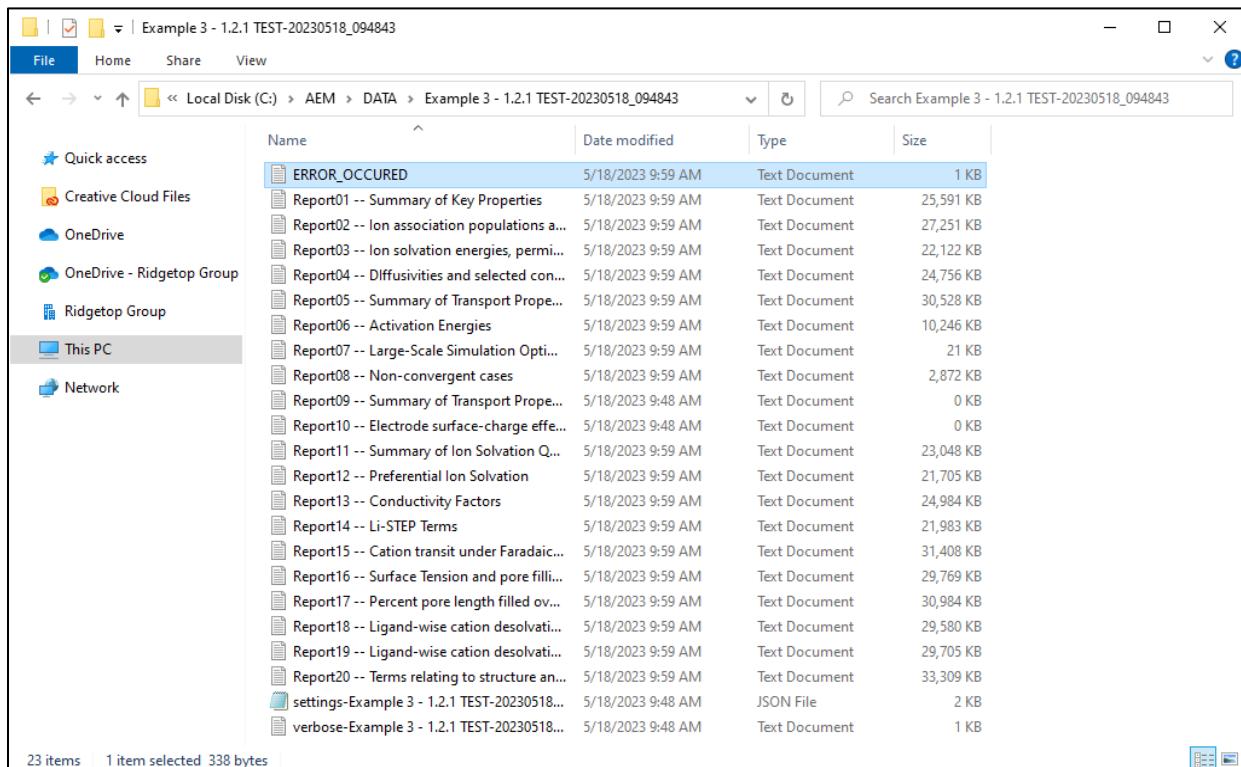
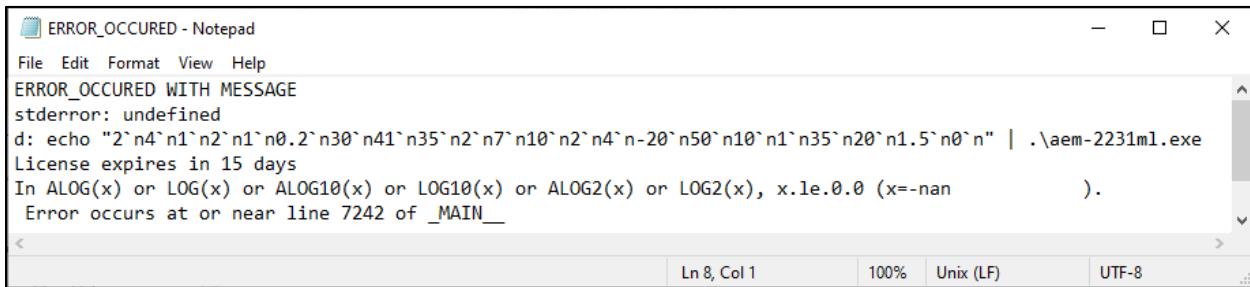


Figure 40. **ERROR\_OCCURRED.txt** located at **C:\Users\user-name\Documents\AEM\DATA\[Simulation Folder Name]**.

## Advanced Electrolyte Model (AEM)



The screenshot shows a Windows Notepad window with the title "ERROR\_OCCURRED - Notepad". The menu bar includes File, Edit, Format, View, and Help. The main content area displays the following text:

```
ERROR_OCCURRED WITH MESSAGE
stderr: undefined
d: echo "2`n4`n1`n2`n1`n0.2`n30`n41`n35`n2`n7`n10`n2`n4`n-20`n50`n10`n1`n35`n20`n1.5`n0`n" | .\aem-2231ml.exe
License expires in 15 days
In ALOG(x) or LOG(x) or ALOG10(x) or LOG10(x) or ALOG2(x) or LOG2(x), x.le.0.0 (x=-nan      ).
Error occurs at or near line 7242 of _MAIN_
```

The status bar at the bottom indicates Ln 8, Col 1, 100%, Unix (LF), and UTF-8.

**Figure 41. ERROR\_OCCURRED.txt as viewed in a Text Editor.**

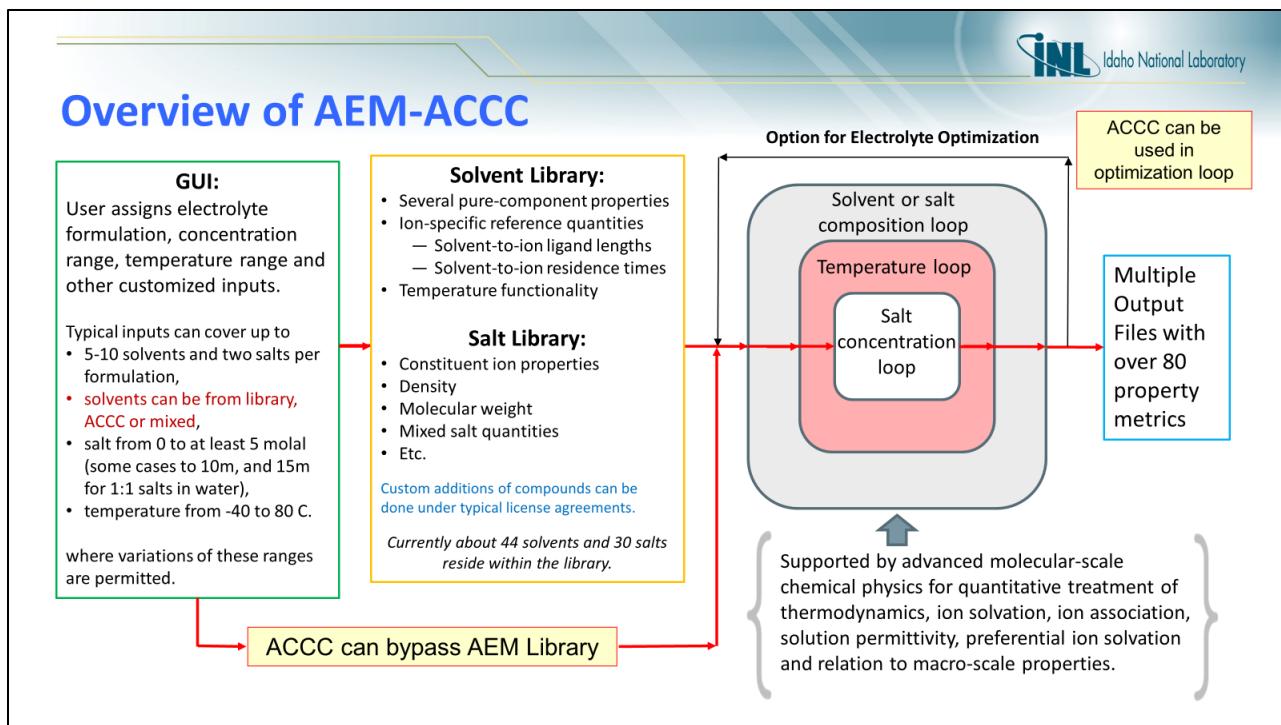
### 3.3 AEM Arbitrarily Chosen Chemical Compounds (ACCC) Module

The Advanced Electrolyte Model (AEM) has long been recognized as a groundbreaking molecular simulation tool by the global battery R&D community, fundamentally transforming the way researchers approach electrolyte chemistry optimization. This robust platform functions as a virtual laboratory, allowing scientists to explore and fine-tune genome-level electrolyte properties with exceptional precision. AEM's comprehensive database includes over 50 solvents and 30 salts, which has consistently demonstrated high accuracy in predicting electrolyte behaviors. By accelerating the adoption of electric vehicles, enabling grid-scale battery systems, and advancing clean energy solutions, AEM plays a vital role in driving the clean energy revolution, guiding global efforts toward a more sustainable future.

Building on this foundation, the new Arbitrarily Chosen Chemical Compounds (ACCC) Module enhances AEM's capabilities by enabling customers to personalize their material libraries with unique salts and solvents. This optional add-on mirrors the functionality seen in the New Chemistry Import Feature for Ridgetop's CellSage Battery Health Modeling, Simulation, and Analysis (MS&A) software platform, where users can upload specific input parameters and baseline testing data to create new cell chemistry models. Both AEM and CellSage are equipped with default libraries that are updated regularly under the term of the customer's Software License Agreement (SLA), but the ACCC Module offers the flexibility to expand these libraries according to their specific research needs and interests. The AEM ACCC Module enables an extensive range of new compounds, significantly enriching the research possibilities within the realms of pure solvents and multi-solvent mixtures.

The reliability of the AEM ACCC Module is underscored by rigorous upfront validation, which confirms that AEM simulations incorporating ACCC definition files achieve targeted results with at least 98% accuracy in conductivity compared to the default simulations using in-code compound parameters. This level of precision is maintained across various applications, including those involving aqueous systems and other complex solvent mixtures. AEM's commitment to accuracy and functionality makes it an indispensable tool in the field of battery research and development, which traditionally suffers from a lack of precise and efficient modeling tools. As the landscape of battery technology evolves rapidly, the need for such advanced tools becomes increasingly critical to understand the complex interactions within batteries and to optimize their electrolyte properties effectively.

As illustrated in Figure 42, the AEM ACCC Module provides a significant enhancement to the capabilities of AEM users. This innovative module allows users to circumvent the standard library of solvents and salts, enabling them to define custom classes of salts and/or solvents. These can then be utilized in electrolyte optimization simulations conducted over various temperature ranges and/or salt concentration gradients. This feature is particularly advantageous for researchers focused on developing new proprietary salts and solvents aimed at creating innovative electrolytes.



**Figure 42. AEM ACCC Overview Diagram.**

The simulation framework employed by the ACCC Module is grounded in advanced molecular-scale chemical physics. It offers a quantitative approach to the thermodynamics, ion solvation, ion associations, solution permittivity, and preferential ion solvation, which are crucial for understanding the relationship between micro-scale chemical interactions and macro-scale properties. This comprehensive framework ensures that simulations are both accurate and relevant to real-world applications.

Furthermore, the AEM ACCC Module includes several detailed data output reports, as discussed in [Section 3.4.2](#) of this User Guide. These reports provide users with deep insights into the outcomes of their simulations, facilitating a thorough analysis of new electrolyte formulations. This level of detail and customization makes the AEM ACCC Module an essential tool for advancing the frontier of electrolyte research.

For customers interested in upgrading their software license to include the AEM ACCC Module, we encourage you to reach out directly to Ridgetop Group or your regional sales representative. Upgrading your software license will unlock these enhanced capabilities, allowing you to leverage the full potential of AEM in your research and development efforts, thereby contributing to the advancement of next-generation energy storage solutions.

### 3.3.1 AEM ACCC Solvent Class

The AEM ACCC Solvent Class, as detailed in Figure 43 and Table 1, is an integral component of the AEM ACCC Module, designed to provide extensive customization in electrolyte simulations. Each solvent within this class is defined by 35 distinct parameters, allowing for precise control over its behavior in simulation environments. These parameters include physical properties such

## Advanced Electrolyte Model (AEM)

as molecular weight, density, viscosity, and dielectric properties, alongside advanced chemical properties like solvation numbers, residence times, and configurational entropy factors. This granular control enables researchers to simulate a wide range of solvent behaviors accurately.

Solvents in the ACCC Solvent Class are defined using unique ACCC solvent definition files, which associate one solvent with one salt, reflecting their specific ion solvation interactions. These solvent definitions are stored in text files (\*.txt), which can be created and managed directly within the AEM graphical user interface (GUI). Once configured, these files can be easily integrated into the AEM GUI or command line interface (CLI) for simulation runs, with the system requiring only one ACCC definition file per simulation. This process is facilitated by a simple suffix system for solvent identification, where solvents such as EP and BN would be labeled as ep.bn or EP-BN in the file name, ensuring a match between user input and filename.

Furthermore, the flexibility of the ACCC Module allows for both ACCC and non-ACCC solvents to be used within the same simulation. This capability enables the use of up to ten ACCC solvents per simulation, significantly broadening the scope for electrolyte formulation. Solvents used in the simulation are flagged within the formulation tables of the output files, providing clear and actionable data for further analysis. This robust framework ensures that AEM users have the tools necessary to push the boundaries of electrolyte chemistry research, paving the way for the development of more efficient and effective energy storage solutions.

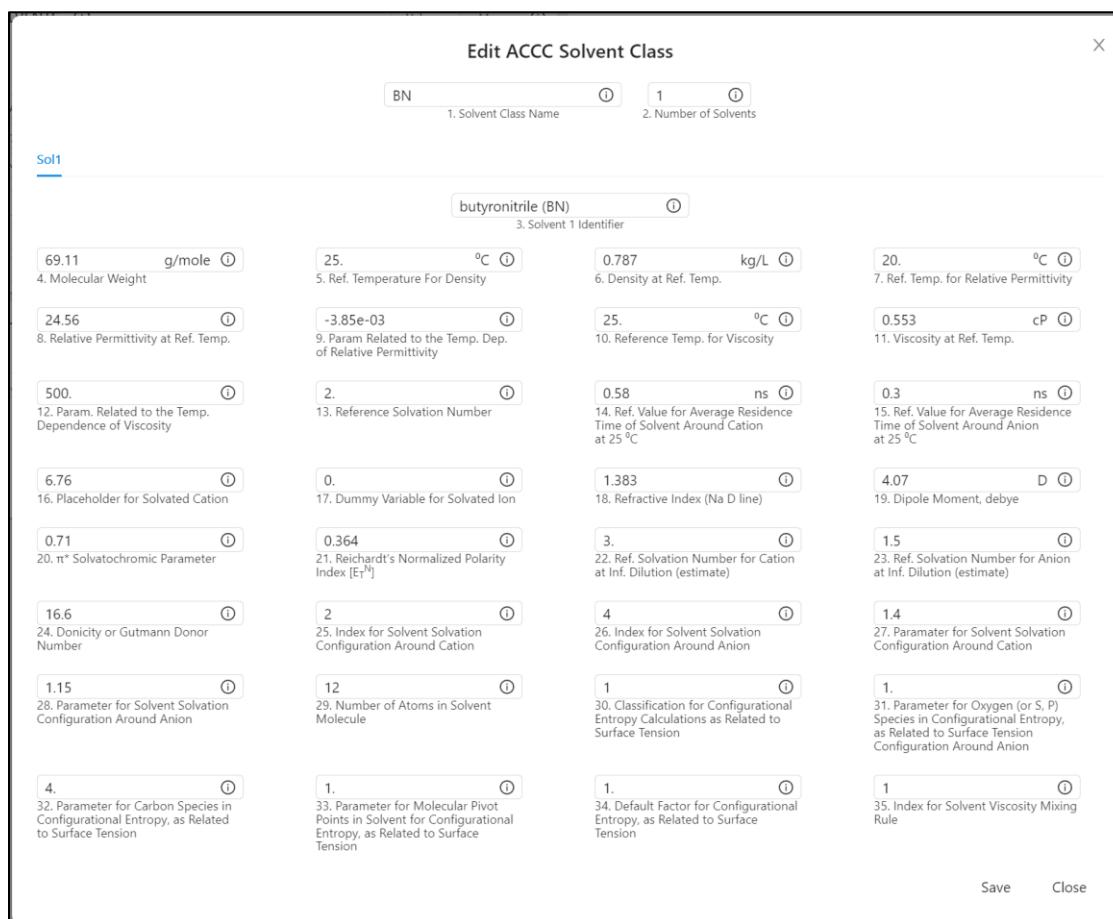


Figure 43. AEM ACCC Solvent Class GUI View.

**Table 1. ACCC Solvent Class Input Parameters.**

ID	Parameter Description	Comments
1	Solvent Class Name	User-defined identifier, Limited to 24 characters
2	Number of Solvents	Limit of 10 depending on the experiment
3	Solvent N Identifier	User-defined identifier
4	Molecular weight, g/mole	Determined experimentally or from online sources (literature, datasets)
5	Reference T for density, degrees C	User defined value
6	Density at reference T, kg/L	Determined experimentally or from online sources (literature, datasets)
7	Reference T for relative permittivity (dielectric constant), degrees C	User defined value
8	Relative permittivity at reference T	Determined experimentally or from online sources (literature, datasets)
9	Parameter related to the temperature dependence of relative permittivity	Slope of d(relative permittivity)/dT on a log basis
10	Reference T for viscosity, degrees C	Determined experimentally or online sources (literature, datasets)
11	Viscosity at reference T, cP	Determined experimentally or online sources (literature, datasets)
12	Parameter related to the temperature dependence of viscosity	This parameter generally falls within values of 200-900. Larger values represent a steeper slope of d(viscosity)/dT.
13	Reference maximum average solvation sites within a single solvent molecule that promote interaction with cations	Estimate of maximum average solvation sites that comprise dipole interactions with a cation, such as lithium, at infinite dilution salt. Values would generally fall within 1 to 6, with common values of 1-3.
14	Reference value for average residence time of solvent around given cation at 25 °C, infinite dilution salt, with units of ns	Key molecular parameters unique to interactions found for each solvent-ion combination. Typically range is 0.5 to 5 ns
15	Reference value for average residence time of solvent around given anion at 25 °C, infinite dilution salt, with units of ns	Key molecular parameters unique to interactions found for each solvent-ion combination. Typical range is 0.2 to 1 ns.
16	Variable for solvated cation	Initial value provided by user (say, 4 to 8 nm); value is updated by code.
17	Variable for solvated ion	Default = 0.
18	Refractive index (Na D line)	Obtained from experiment/simulations; see ACCC examples for common values

19	Dipole moment, Debye	Estimated numerically from similar compounds; see ACCC examples for common values
20	$\pi^*$ solvatochromic parameter	Estimated numerically from similar compounds; see ACCC examples for common values
21	Reichardt's normalized polarity index ( $E_T^N$ )	Estimated numerically from similar compounds; see ACCC examples for common values
22	Reference solvation number for cation at infinite dilution (estimate)	Obtained from experiment/simulations; common range is 2 to 6
23	Reference solvation number for anion at infinite dilution (estimate)	Obtained from experiment/simulations; common range is 0.5 to 2
24	Donicity or Gutmann donor number	Estimated numerically from similar compounds; common range is 10 to 24
25	Index for solvent solvation configuration around cation	Refer to Figure 44.
26	Index for solvent solvation configuration around anion	Refer to Figure 44.
27	Parameter for solvent solvation configuration around cation	Solvent shape variable for solvent in proximity to cation that determines relative scale between major and minor axes. Default = 1, with typical values ranging from 0.5 to 4.
28	Parameter for solvent solvation configuration around anion	Solvent shape variable for solvent in proximity to cation that determines relative scale between major and minor axes. Default = 1, with typical values ranging from 0.5 to 4.
29	Number of atoms in solvent molecule	Obtained from solvent molecule description
30	Classification for configurational entropy calculations, as related to surface tension	'1' (default) when pivot-point carbons are used '2' when total free carbons are used
31	Parameter for oxygen (or S, P) species in configurational entropy, as related to surface tension	Number of (O, S, P) in molecule
32	Parameter for carbon species in configurational entropy, as related to surface tension	Number of C in molecule
33	Parameter for molecular pivot points in solvent for configurational entropy, as related to surface tension	Number of "pivot points" in molecular structure that enable increased configurational entropy.

34	Default factor for configurational entropy, as related to surface tension	Default value of '1'.
35	Index for solvent viscosity mixing rule	Most systems at '1', PC-based at '2', glyme-based at '3'. This assigns which set of viscosity mixing parameters are used for a pure solvent mixture.

Additional Notes for ACCC Solvent Class:

1. For Parameters with a Green ID, these values are typically known or easily derived.
2. For Parameters with a Red ID, these values are typically unknown but, in many cases, can be estimated from similar compounds. This requires some level of iteration to satisfy model accuracy for an array of properties.
3. For Parameters 17-25, these values will be unique to the chosen salt, and require some level of optimization to get accurate ion solvation characterization and numerous other properties.
4. For Parameters 25-28, these are key parameters for solvated ion molecular configurations based on average solvent-ion interactions. Unique to each solvent-ion combination at 25 °C, infinite dilution.
5. For Parameters 30-35, these parameters are part of a proprietary algorithm developed by Idaho National Laboratory.
6. Figure 44 refers to the options tied to parameters 25 and 26.

**Time-averaged Ion Solvation Configuration Options for necc1 (cation) and necc2 (anion):**

n = 1 -- spherical solvent molecule (default)		<p>Solvent-to-ion alignment shown here as right-to-left:</p> <p>n = 1      </p> <p>n = 2      </p> <p>n = 6      </p> <p>etc.</p> <p>for ion as </p> <p>Shape variables erecc1 (cation) and erecc2 (anion) determine relative scale between major and minor axes:</p> <p></p> <p></p>
n = 2 -- ellipsoidal solvent oriented toward ion along major axis		
n = 3 -- ellipsoidal solvent oriented toward ion along minor axis.....		
n = 4 -- elliptical paraboloid solvent oriented toward ion along major axis		
n = 5 -- elliptical paraboloid solvent oriented toward ion along minor axis		
n = 6 -- average of spherical and ellipsoidal/major		
n = 7 -- average of spherical and ellipsoidal/minor.....		
n = 8 -- average of spherical and elliptical paraboloid/major		
n = 9 -- average of spherical and elliptical paraboloid/minor		
n = 10 -- average of ellipsoidal/major and elliptical paraboloid/major.....		
n = 11 -- average of ellipsoidal/minor and elliptical paraboloid/major		
n = 12 -- average of ellipsoidal/major and elliptical paraboloid/minor		
n = 13 -- average of ellipsoidal/minor and elliptical paraboloid/minor		
n = 14 -- reverse of elliptical paraboloid solvent oriented toward ion along major axis (mostly for anions)		

**Figure 44. Note for time-average ion solvation.**

## Advanced Electrolyte Model (AEM)

### 3.3.2 Example of AEM ACCC Solvent Class

The Advanced Electrolyte Model (AEM) has introduced an innovative approach for simulating solvent interactions within electrolytes through its Arbitrarily Chosen Chemical Compounds (ACCC) Module. This section of the User Guide highlights the Solvent Examples used to test and validate this module. A comprehensive set of 16 Solvent Definition files were developed, showcasing the module's robustness and versatility. Figures 45 offers a visual reference for users to better understand the configuration and application of the ACCC Solven Class within AEM.

Edit ACCC Solvent Class

BN      1

Sol1

BN	Solvent Class Name	1	Number of Solvents
butyronitrile (BN)	Solvent 1 Identifier		
69.11 g/mole	25. °C	0.787 kg/L	20. °C
Molecular Weight	Ref. Temperature For Density	Density at Ref. Temp.	Ref. Temp. for Relative Permittivity
24.56	-3.85e-03	25. °C	0.553 cP
Relative Permittivity at Ref. Temp.	Param Related to the Temp. Dep. of Relative Permittivity	Reference Temp. for Viscosity	Viscosity at Ref. Temp.
500.	2.	0.58 ns	0.3 ns
Param. Related to the Temp. Dependence of Viscosity	Reference Solvation Number	Ref. Value for Average Residence Time of Solvent Around Cation at 25 °C	Ref. Value for Average Residence Time of Solvent Around Anion at 25 °C
6.76	0.	1.383	4.07 D
Placeholder for Solvated Cation	Dummy Variable for Solvated Ion	Refractive Index (Na D line)	Dipole Moment, debye
0.71	0.364	3.	1.5
π <sup>x</sup> Solvatochromic Parameter	Reichardt's Normalized Polarity Index [E <sub>r</sub> <sup>N</sup> ]	Ref. Solvation Number for Cation at Inf. Dilution (estimate)	Ref. Solvation Number for Anion at Inf. Dilution (estimate)
16.6	2	4	1.4
Donicity or Gutmann Donor Number	Index for Solvent Solvation Configuration Around Cation	Index for Solvent Solvation Configuration Around Anion	Paramater for Solvent Solvation Configuration Around Cation
1.15	12	1	1.
Parameter for Solvent Solvation Configuration Around Anion	Number of Atoms in Solvent Molecule	Classification for Configurational Entropy Calculations as Related to Surface Tension	Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion
4.	1.	1.	1.
Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	Default Factor for Configurational Entropy, as Related to Surface Tension	Index for Solvent Viscosity Mixing Rule

Save      Close

**Figure 45. ACCC Solvent Definition for Butyronitrile (BN).**

Figure 155 through Figure 169 in [Section 7.2](#) of the Appendix provide detailed screenshots for other ACCC solvent examples. The selection of solvents for the ACCC Module was influenced by existing solvent types already integrated into AEM, ensuring a seamless validation and demonstration process. The focus was on organic carbonates, esters, and nitriles, with specific examples including ethylene carbonate (EC), propylene carbonate (PC), dimethyl carbonate (DMC), methyl acetate (MA), ethyl acetate (EA), and acetonitrile (AN), among others. Additionally, optional solvents such as dimethoxyethane (DME), diglyme, and water were also considered.

These choices reflect the diversity and flexibility of the AEM in handling various solvent types, enhancing the accuracy and applicability of the model in real-world scenarios.

In terms of technical details, each ACCC solvent definition within the module contains 35 distinct parameters, meticulously defined to capture the unique ion solvation behaviors of different solvent-salt combinations. This is exemplified by the Solvent-LiPF<sub>6</sub> definition file, which are specifically highlighted for their precision in mimicking real electrolyte behaviors. The ACCC solvent definition files are stored in text files (\*.txt) which are automatically recognized and processed by the AEM software program when properly assigned by the user. Although the ACCC solvent definition files can be edited in a text editor program, it is recommended that each solvent definition is edited using the AEM GUI.

The integration of ACCC and non-ACCC solvents within the same simulation is a testament to the model's flexibility, allowing for a wide range of electrolyte formulations. This capability supports the use of anywhere from 0 to 10 ACCC solvents in a single simulation, significantly expanding the experimental scope. Solvents involved in the simulations are flagged within the formulation tables of the output files, ensuring clear and accessible data for analysis. This level of detail and accuracy, with simulation results matching the default simulations to an accuracy of  $\geq 99\%$  based on conductivity, confirms the efficacy of the AEM-ACCC functionality in advancing electrolyte research and application.

### **3.3.3 AEM ACCC Salt Class**

The AEM ACCC Salt Class, detailed in Figure 46 and Table 2, enriches the AEM compound library by providing a specialized framework for the precise characterization of salts used in electrolyte simulations. This class encompasses 23 distinct parameters for each salt, enabling a deep dive into the ion solvation behaviors that are critical for understanding and optimizing electrolyte formulations.

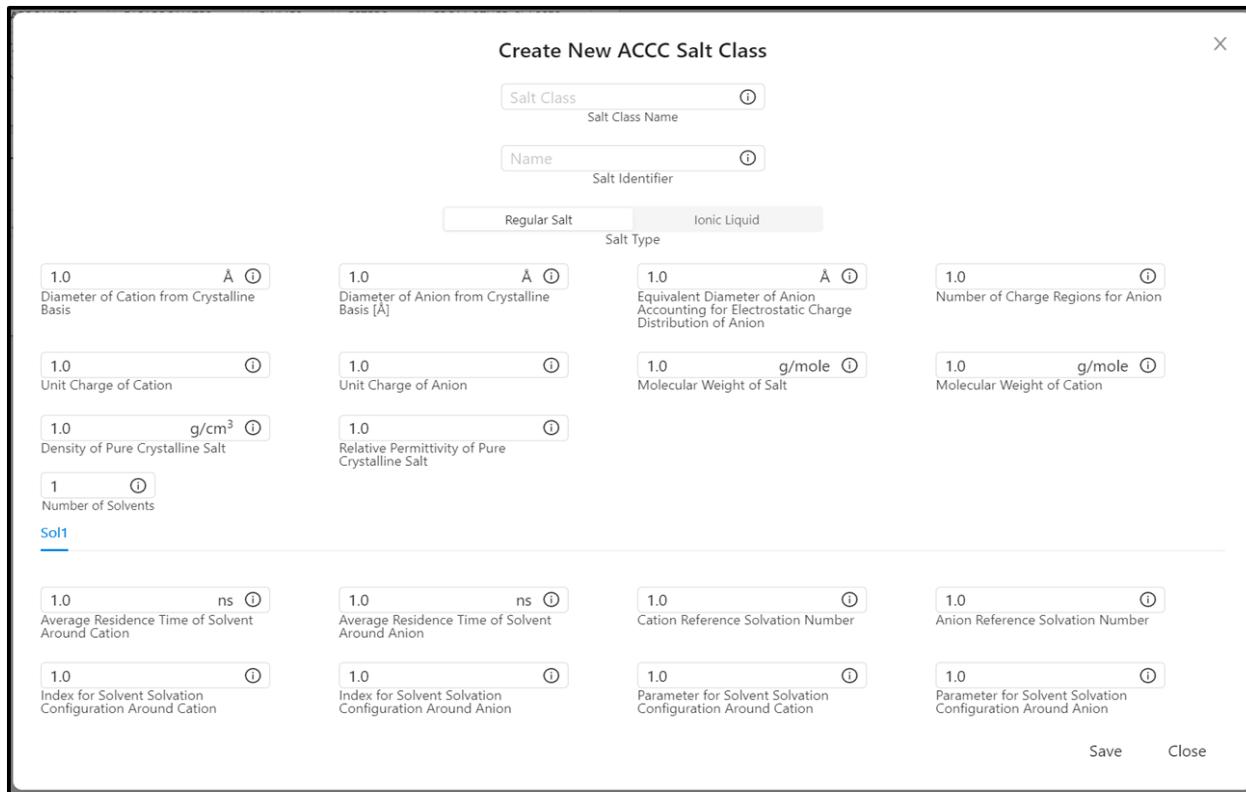
In the ACCC Salt Class, each salt is defined in conjunction with one or more solvents, capturing the unique solvation interactions specific to each salt-solvent combination. This is facilitated through the use of ACCC salt definition files, which are text files (\*.txt) created and managed within the AEM graphical user interface (GUI). Once these files are set up, they are seamlessly integrated into the AEM GUI or command-line interface (CLI) for simulation purposes. Additionally, a corresponding ACCC solvent file may be included in the simulation as needed.

Salt assignment within the AEM system is straightforward, requiring users to input a simple suffix when prompted by the software. For instance, a salt like LiPF<sub>6</sub> used in an electrolyte combination with EC, DMC, and MP would have a suffix like LiPF<sub>6</sub>\_w\_EC\_DMC\_MP, and all relevant ACCC data for this setup would be stored in a file named ACCC Inputs (Salt Class)--LiPF<sub>6</sub>\_w\_EC\_DMC\_MP.txt. It is crucial that the suffix provided matches exactly between the user input and the filename to ensure proper file handling and simulation accuracy.

The ACCC framework supports the use of both ACCC and non-ACCC salts within the same simulation, allowing researchers greater flexibility in designing electrolyte formulations. This capability is particularly advantageous as it accommodates the inclusion of up to one ACCC salt per simulation, enhancing the adaptability of the AEM to meet diverse research needs. In the

## Advanced Electrolyte Model (AEM)

output files, ACCC salts are distinctly flagged within the formulation tables, providing clear visibility and ease of analysis for researchers evaluating the impacts of different salt configurations on the electrolyte's performance. This comprehensive approach ensures that the AEM ACCC Salt Class is a robust tool for advancing the field of electrolyte chemistry.



**Figure 46. AEM ACCC Salt Class GUI View.**

**Table 2. ACCC Salt Class Input Parameters.**

ID	Parameter Description	Comments
1	Salt Class Name	User-defined identifier, limited to 25 characters
2	Salt Identifier	Salt name, limited to 12 characters
3	Salt Type	'1' – regular salts '2' – ionic liquids
4	Diameter of cation from crystalline basis, Angstrom	Obtained from Pauling radii
5	Diameter of anion from crystalline basis, Angstrom	Obtained from Pauling radii
6	Equivalent diameter of anion accounting for electrostatic charge distribution of anion, Angstrom (this term $\leq$ sig2p)	If anion has a localized charge, then estimate the effective diameter of the solvent defined at that charge locus, considering the closest approach to charge.
7	Number of charge regions for a given anion (default value = 1.; value	default value = 1.; value of 2 or higher used for non-uniform acentric charge.

## Advanced Electrolyte Model (AEM)

	of 2. or higher used for non-uniform acentric charge)	Use default value for simple anions where the effective electrostatic anion diameter is the same as the cryst. value . A value of 2 may be warranted for more complex anions.
8	Unit charge of cation	Positive integers 1, 2, 3 etc.
9	Unit charge of anion	Negative integers -1, -2, -3 etc.
10	Molecular weight of salt	Obtained from experiment/online sources
11	Molecular weight of cation	Obtained from experiment/online sources
12	Density of pure crystalline salt, subtracting void space contribution from particle packing fraction, g/cm <sup>3</sup> .	Obtained from experiment/online sources
13	Relative permittivity of pure crystalline salt	Obtained from experiment/online sources. Typical values range from 10-20.
14	Factor to express equivalent diameter of cation in RTIL accounting for electrostatic charge distribution of cation, Angstrom (this term between 0 to 1)	Accounts for charge dislocation and corresponding reduced electrostatic diameter of the cationic member of the RTIL. Theoretical values range from 0. to 1., with a practical range of 0.5 to 1.
15	Number of charge regions for a given cation in RTIL (default value = 1.; value of 2. or higher used for non-uniform acentric charge)	Analogous to Item 7 herein.  (Default value = 1.; value of 2. or higher used for non-uniform acentric charge)
16	Reference value for average residence time of solvent around given cation at 25 °C, infinite dilution, ns	Key molecular parameters unique to interactions found for each solvent-ion combination. Typical range is 0.2 to 1 ns.
17	Reference value for average residence time of solvent around given anion at 25 °C, infinite dilution, ns	Initial value provided by user (say, 4 to 8 nm); value is updated by code.
18	Reference solvation number for cation at infinite dilution (estimate)	Obtained from experiment/simulations; common range is 2 to 6
19	Reference solvation number for anion at infinite dilution (estimate)	Obtained from experiment/simulations; common range is 0.5 to 2
20	Index for solvent solvation configuration around cation	Refer to Figure 44.
21	Index for solvent solvation configuration around anion	Refer to Figure 44.
22	Parameter for solvent solvation configuration around cation	Solvent shape variable for solvent in proximity to cation that determines relative scale between

		major and minor axes. Default = 1, with typical values ranging from 0.5 to 4.
23	Parameter for solvent solvation configuration around anion	Solvent shape variable for solvent in proximity to cation that determines relative scale between major and minor axes. Default = 1, with typical values ranging from 0.5 to 4.

Additional Notes for ACCC Salt Class:

1. For Parameters 16-23, these terms were discussed in the previous section for the ACCC Solvent Class.
2. Note that if an ACCC solvent and an ACCC salt are both used in a simulation, these terms must be identical within the two input definition files / strings covering the ACCC solvent and salt.

### 3.3.4 Example of AEM ACCC Salt Class

The Advanced Electrolyte Model (AEM) has further extended its functionality with the Arbitrarily Chosen Chemical Compounds (ACCC) Module, which includes a detailed implementation of salt definitions to enhance simulation capabilities. To validate this aspect of the module, six Salt Definition files were meticulously developed, encompassing a variety of commonly used lithium salts and ionic liquids. Figures 63 provides a visual demonstration for one example salt definition file, aiding users in comprehending the specific configurations and applications within the model. Figure 171 through Figure 175 in [Section 7.3](#) of the Appendix shows additional examples for each of the default ACCC salt definition files that were tested and validated. The salts tested include LiPF6, LiFSI, LiTFSI, LiBOB, LiAsF6, and LiBF4, alongside room temperature ionic liquids (RTILs) such as PYR13-FSI and EMI-FSI.

Each salt in the ACCC Module is parameterized with 23 unique values that reflect its ion solvation behavior, which is crucial for accurately simulating the interaction between salts and solvents. The individual ACCC salt definitions are strategically structured to define interactions between a specific salt and one or more solvents, capturing the unique characteristics of each combination. This detailed approach ensures that the simulation results are highly accurate, achieving an impressive  $\geq 98\%$  accuracy compared to default simulations that use built-in parameters, particularly noting the efficiency in simulating non-aqueous systems.

The flexibility of the AEM in handling various salt and solvent combinations is showcased through the capability to read and integrate ACCC salt definition files, which are stored as text files (\*.txt) and are automatically recognized by the AEM once proper assignments are made. This process involves assigning a specific suffix when prompted by the software, which directs the model to the appropriate file containing all necessary ACCC data. For instance, if an electrolyte simulation involves LiPF6 with solvents like ethylene carbonate (EC), dimethyl carbonate (DMC), and methyl propionate (MP), the user would input the suffix 'LiPF6\_w\_EC\_DMC\_MP', correlating exactly with the filename 'ACCC Inputs (Salt Class)--LiPF6\_w\_EC\_DMC\_MP.txt'.

Moreover, the AEM allows for the integration of both ACCC and non-ACCC salts in the same simulation, offering a broader range of electrolyte formulations to researchers. This inclusion can

## Advanced Electrolyte Model (AEM)

accommodate either zero or one ACCC salt per simulation, enhancing the model's adaptability to various research needs. All salts, whether ACCC or not, are clearly flagged in the formulation tables within the output files, providing an easy reference for analyzing the results. This comprehensive system ensures that users can efficiently manipulate and utilize the AEM for advanced simulations, pushing the boundaries of electrolyte research.

### Edit ACCC Salt Class

LiBF4\_w\_EC\_EMCSalt Class Name

LiBF4Salt Identifier

Regular Salt Ionic LiquidSalt Type

1.36 Å Diameter of Cation from Crystalline Basis	3.795 Å Diameter of Anion from Crystalline Basis [Å]	3.795 Å Equivalent Diameter of Anion Accounting for Electrostatic Charge Distribution of Anion	1. Number of Charge Regions for Anion
1. Unit Charge of Cation	-1. Unit Charge of Anion	93.74 g/mole Molecular Weight of Salt	6.941 g/mole Molecular Weight of Cation
2.15 g/cm³ Density of Pure Crystalline Salt	16. Relative Permittivity of Pure Crystalline Salt		
2 Number of Solvents			
Sol1	Sol2		
0.357 ns Average Residence Time of Solvent Around Cation	0.7 ns Average Residence Time of Solvent Around Anion	4. Cation Reference Solvation Number	2. Anion Reference Solvation Number
10 Index for Solvent Solvation Configuration Around Cation	4 Index for Solvent Solvation Configuration Around Anion	1.28 Parameter for Solvent Solvation Configuration Around Cation	2.2 Parameter for Solvent Solvation Configuration Around Anion

Save Close

**Figure 47. ACCC Salt Definition for LiBF4\_w\_EC\_EMCS.**

### 3.3.5 Example of ACCC Validation

This section demonstrates two example validation cases for the ACCC module, considering both cases of solvent and salts that are defined as an ACCC class. Additional validation cases for other solvents and salts can be reviewed in [Section 7.4](#) of the Appendix. As shown in Figure 48 and Figure 49, the validation process involved conducting two simulations: the first using the default library with non-ACCC solvent or salt compounds (represented by the black curves in the figures), and the second using the same compounds defined as ACCC solvents or salts (represented by the red-dashed curves in the figures). The results, focusing on electrolyte conductivity, indicate that the accuracy remains high between ACCC and non-ACCC cases, showing no significant differences in outcomes between the two methods. The agreement is generally within 99% accuracy for library versus ACCC bases, demonstrating that ACCC effectively bypasses the library. This consistency across various solvent and salt types indicates that the system's performance is robust and repeatable with the ACCC architecture.

### Advanced Electrolyte Model (AEM)

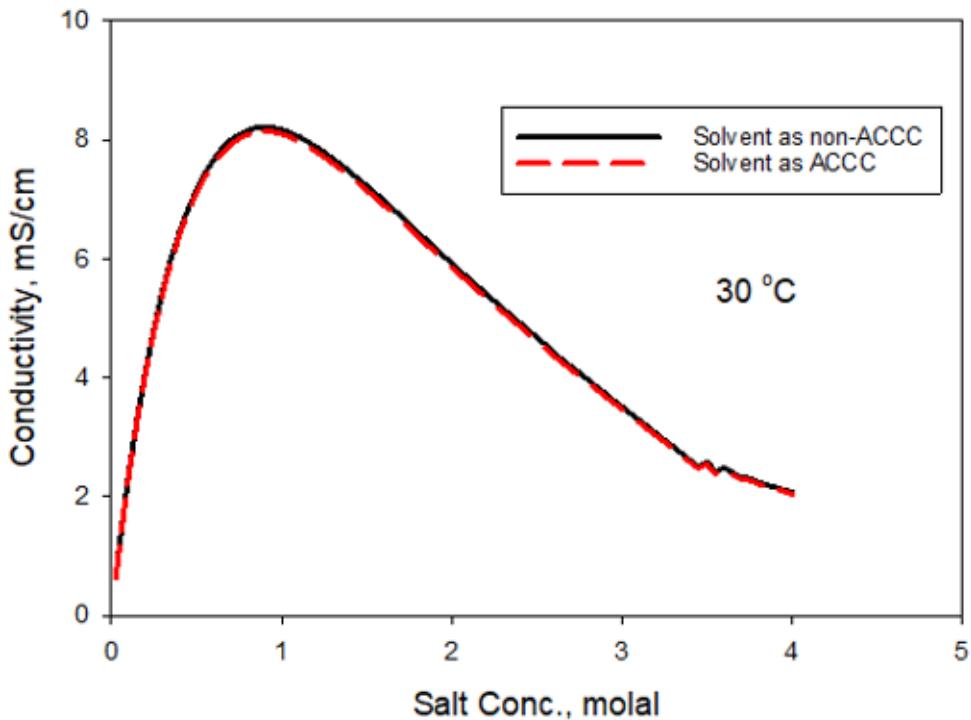


Figure 48. EC+LiPF<sub>6</sub> at 30°

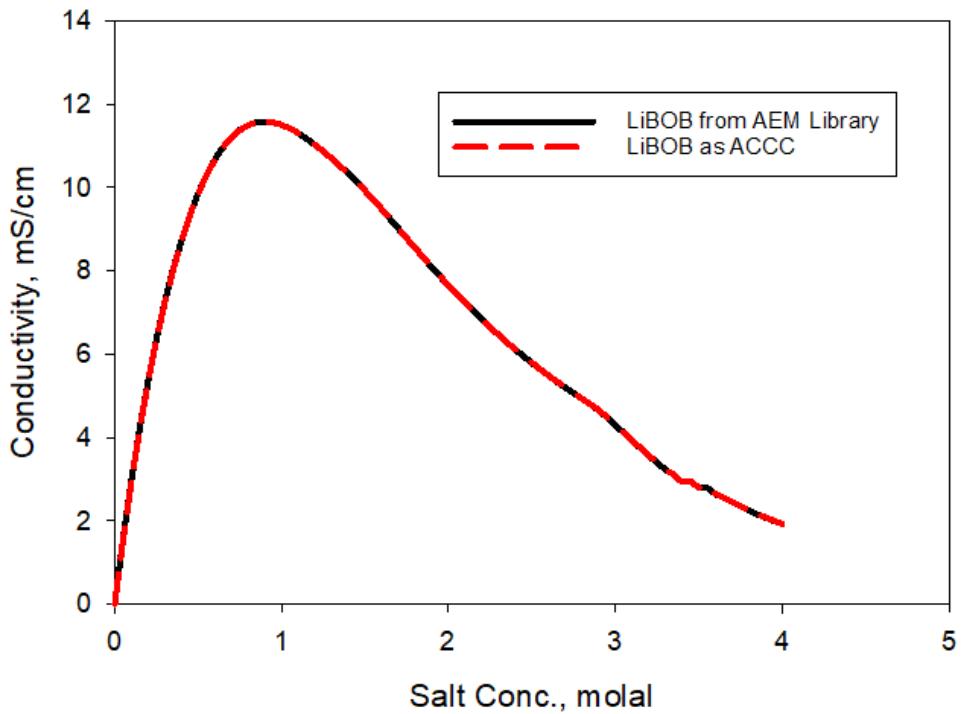


Figure 49. PC-EA (3:7 by mass) + LiBOB

## 3.4 AEM Output Tab

The second and final tab in the AEM GUI is the **AEM Output** tab, where the user can preview input conditions for a particular run, toggle between multiple different runs, and view data output records and plots for each individual run. The **AEM Output tab** is separated into the following components.

- Sidebar that contains three select drop-down sections – **AEM RUNS**, **AEM REPORTS**, **Data Display** and a text previewing window in the **AEM RUNS** section.
- **REPORT TEXT** section with a text viewer scroll box.
- **REPORT DATA VISUALIZATION** section with three select drop down sections – **Filter List**, **X-Axis Parameter**, **Y-Axis Parameter**, a list scroll box to display options based on what filter is chosen in the **Filter List** section, and a graphing chart to display output data plots based on what is chosen in the **X-Axis Parameter** and **Y-Axis Parameter** sections.

A visual of the AEM Output Tab with the **REPORT TEXT** section (Figure 50) and **REPORT DATA VISUALIZATION** section (Figure 51) is shown below.

The screenshot shows the AEM Output tab interface. On the left, there's a sidebar with 'AEM Input' and 'AEM Output' tabs. Under 'AEM Input', there's a dropdown menu set to 'Example 1-20230516\_114210'. The 'AEM Output' tab is active. It has three dropdown menus: 'Mode: Fixed', 'Solvent Comp. Proportionality Basis: Volume', and 'Solvents: Ethyl Propionate (EP) Volume: 25, Dimethyl Carbonate (DMC) Volume: 50, Ethylene Carbonate (EC) Volume: 25'. Below these are sections for 'Salt': 'LiPF6', 'Max Total Salt Concentration: 5 molal', 'Temperature Min: 30°C', 'Temperature Max: 40°C', 'Temperature Step Size: 1°C', 'Ion Stability Method: Option 1', 'Contact Angle: 35°', 'Total Pore Length: 20µm', 'Salt Concentration of Interest: 1.5 molal', 'SCAP Calculations: false', and 'Double Layer Calculations: false'. The 'AEM REPORTS' dropdown is set to 'Report01 -- Summary of Key Properties.txt'. The 'Data Display' dropdown is set to 'Text'. The main area is titled 'REPORT TEXT' and contains the following text:

```

AEM ver. 2.23.1M
*** CALCULATIONS ARE PERFORMED ACCOUNTING FOR THE EFFECT OF ION ASSOC. ON HSA PARAMETERS AND OTHER QUANTITIES.

Number of Mixed-Salt Mole Fraction Cases = 1
k1,k2,k3,k4,ksum = 1 0 0 0 1

Results for salt = LiPF6      at Temp. = -40.00 C or -40.00 F, and 1/T(K) = 0.004289
-----
Solvent composition (salt-free):
  Name          Mole Fraction   Mass Fraction   Volume Fraction
ethylene carbonate    0.33980    0.38773    0.25318
dimethyl carbonate    0.45743    0.48899    0.49993
ethyl propionate     0.18271    0.20364    0.24692
-----

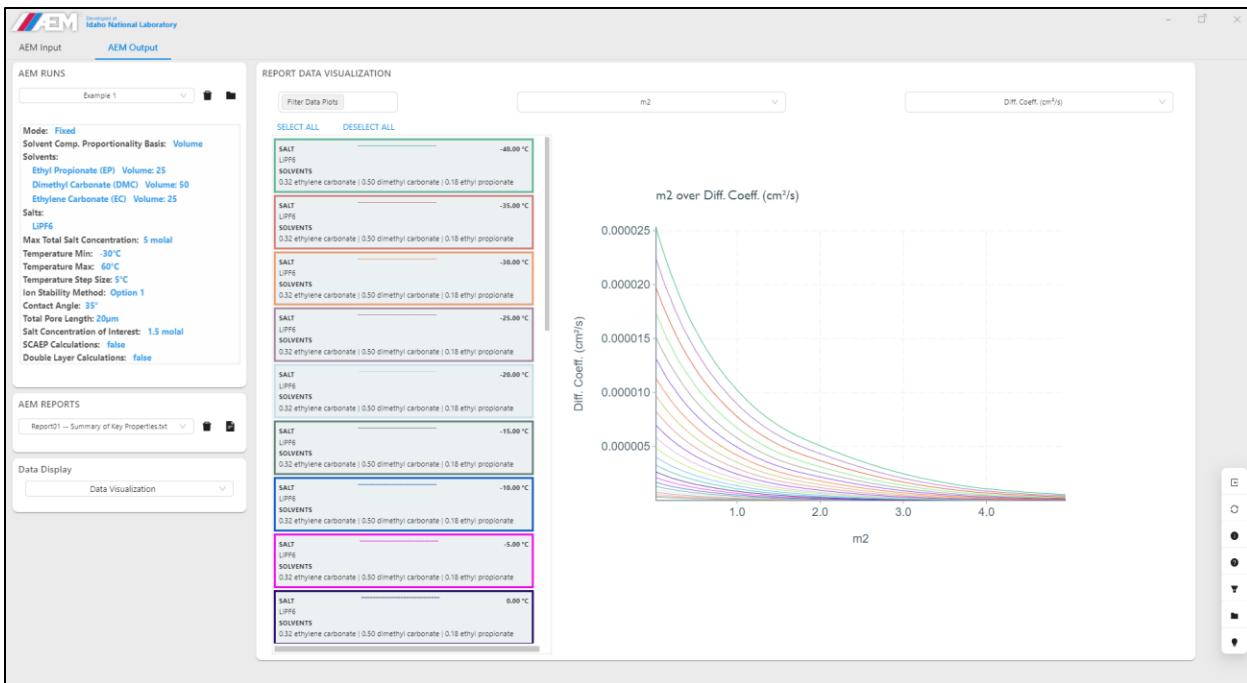
```

Below this is a large table of data:

m <sub>2</sub>	c <sub>2</sub>	wt fr salt	mole fr salt	density (g/cc)	visc. (cP)	Sigf (a <sup>ff</sup> )	Sig2 (a <sup>ff</sup> )	S(+) yr <sup>-1</sup>	Rational Act. Coef.	Diff. Coef.	Spec. Cond. (mS/cm)	t+(a)	t+(b)	dissoc (SI)	dissoc (T)
0.025	0.025	0.004	0.002	1.163	3.98	8.153	7.131	3.945	0.5895e+00	0.2395e-06	0.1735e+00	0.388	0.388	0.59959	0.00000
0.100	0.100	0.015	0.009	1.163	4.21	8.156	7.126	3.945	0.5895e+00	0.2395e-06	0.1735e+00	0.388	0.388	0.59959	0.00000
0.115	0.115	0.015	0.009	1.168	4.46	8.139	7.126	3.969	0.4606e+00	0.2666e-06	0.640e+00	0.385	0.385	0.59959	0.00000
0.150	0.172	0.022	0.014	1.172	4.81	8.131	7.122	3.984	0.4346e+00	0.2466e-06	0.5096e+00	0.388	0.388	0.59959	0.00000
0.200	0.226	0.035	0.020	1.177	5.27	8.121	7.120	3.998	0.4126e+00	0.2256e-06	0.4126e+00	0.391	0.391	0.59981	0.00001
0.250	0.285	0.037	0.022	1.182	5.57	8.114	7.112	4.009	0.4225e+00	0.2116e-06	0.1377e+01	0.395	0.395	0.59981	0.00001
0.300	0.348	0.044	0.027	1.187	5.98	8.104	7.106	4.020	0.4227e+00	0.1968e-06	0.1568e+01	0.398	0.398	0.59973	0.00002
0.350	0.406	0.050	0.031	1.193	6.42	8.086	7.096	4.030	0.4226e+00	0.1822e-06	0.1762e+01	0.401	0.401	0.59973	0.00002
0.400	0.451	0.057	0.035	1.196	6.58	8.066	7.092	4.038	0.4245e+00	0.1787e-06	0.1875e+01	0.403	0.403	0.59953	0.00006
0.450	0.506	0.064	0.045	1.200	7.41	8.076	7.085	4.044	0.4756e+00	0.1588e-06	0.1998e+01	0.408	0.408	0.59939	0.00009
0.500	0.568	0.071	0.044	1.205	7.96	8.065	7.077	4.049	0.5025e+00	0.1476e-06	0.2108e+01	0.409	0.409	0.59922	0.00014
0.550	0.634	0.078	0.049	1.210	8.26	8.056	7.068	4.054	0.5356e+00	0.1364e-06	0.2218e+01	0.411	0.411	0.59909	0.00020
0.600	0.668	0.084	0.052	1.214	9.22	8.045	7.060	4.054	0.5736e+00	0.1276e-06	0.2256e+01	0.415	0.415	0.59874	0.00029
0.650	0.721	0.096	0.056	1.219	9.94	8.035	7.051	4.055	0.6186e+00	0.1176e-06	0.2296e+01	0.418	0.418	0.59842	0.00042
0.700	0.774	0.106	0.062	1.223	10.62	8.025	7.042	4.056	0.6636e+00	0.1076e-06	0.2336e+01	0.421	0.421	0.59812	0.00060
0.750	0.826	0.102	0.064	1.228	11.63	8.013	7.034	4.051	0.7366e+00	0.1006e-06	0.2346e+01	0.424	0.424	0.59764	0.00080
0.800	0.879	0.108	0.068	1.232	12.63	8.003	7.024	4.046	0.8116e+00	0.9256e-07	0.2336e+01	0.427	0.427	0.59720	0.00107
0.850	0.931	0.114	0.072	1.236	13.74	7.992	7.015	4.040	0.8996e+00	0.8506e-07	0.2311e+01	0.429	0.429	0.59666	0.00143
0.900	0.983	0.120	0.078	1.241	14.91	7.981	7.006	4.034	0.9916e+00	0.7756e-07	0.2286e+01	0.432	0.432	0.59591	0.00191
0.950	1.034	0.126	0.088	1.245	16.39	7.971	6.996	4.012	0.1126e+01	0.7146e-07	0.2226e+01	0.435	0.435	0.59511	0.00254
1.000	1.085	0.132	0.088	1.249	17.99	7.968	6.986	4.000	0.1265e+01	0.6516e-07	0.2168e+01	0.438	0.438	0.59402	0.00338
1.050	1.135	0.138	0.088	1.254	19.79	7.958	6.976	3.987	0.1436e+01	0.5926e-07	0.2096e+01	0.440	0.440	0.59267	0.00445

Figure 50. Tab 1 – AEM Output with REPORT TEXT section.

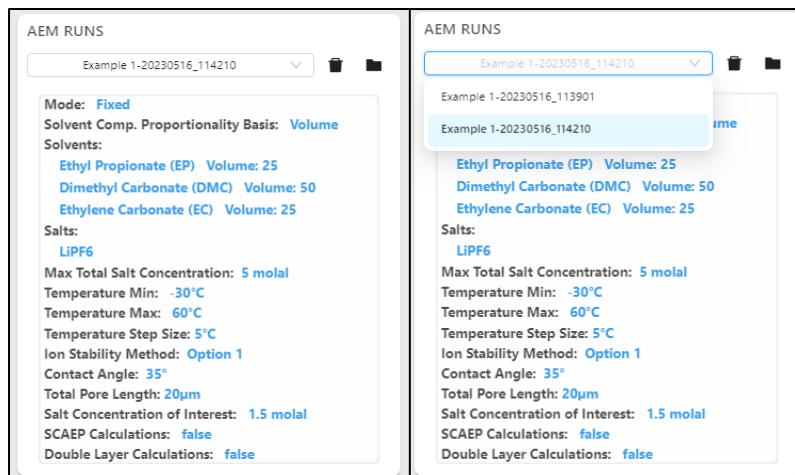
## Advanced Electrolyte Model (AEM)



**Figure 51. Tab 1 – AEM Output with REPORT DATA VISUALIZATION section.**

### 3.4.1 AEM RUNS

This is a dropdown select option where the user can access a list of available simulation runs that have been logged in the data output directory - **C:\Users\user-name\Documents\AEM\DATA\**. The GUI also provides a text previewing window to preview a full set of simulation conditions from a .json file that is stored in the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory. The user can use the **Delete** button (>Delete) to delete the instance for a particular run and the **Reveal in File Explorer** button (>Reveal) to open the .json file in File Explorer on the user's local machine. A visual of this section is shown in Figure 52 below.



**Figure 52. AEM RUNS section of the AEM Output tab.**

### 3.4.2 AEM REPORTS

When all the simulations settings are supplied and the user clicks on the **Run AEM** button on the **AEM Input** tab, AEM starts the simulation run. It then updates the output report files with the simulation results. The user can choose to run the simulation with another set of conditions. The results of a subsequent simulation run will be appended to the output files. However, if the software is restarted, then those files will be overwritten. These files should be copied to another folder for future use. The next simulation run will overwrite any results in these files. The following output report files are created as a result. These are described in section 7.1 later in detail.

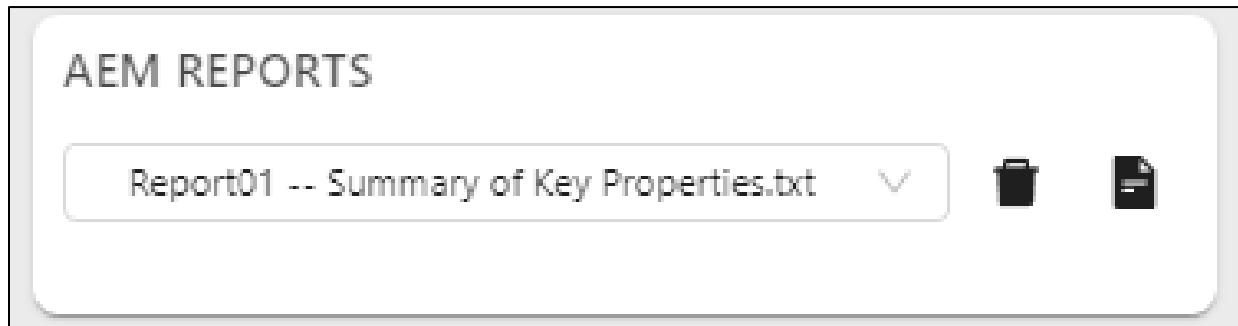
- ◆ **Report1** -- Summary of Key Properties
- ◆ **Report2** -- Ion association populations and other thermodynamic terms
- ◆ **Report3** -- Ion solvation energies, permittivity and cation desolvation
- ◆ **Report4** -- Diffusivities and selected conductivity terms
- ◆ **Report5** -- Summary of Transport Properties and Walden analysis
- ◆ **Report6** -- Activation Energies
- ◆ **Report7** -- Large-Scale Simulation Optimization
- ◆ **Report8** -- Non-convergent cases
- ◆ **Report9** -- Double-Layer Regions transport analysis
- ◆ **Report10** -- Electrode surface-charge effects
- ◆ **Report11** -- Summary of Ion Solvation Quantities
- ◆ **Report12** -- Preferential Ion Solvation
- ◆ **Report13** -- Conductivity Factors
- ◆ **Report14** -- Li-STEP Terms
- ◆ **Report15** -- Cation transit under Faradaic conditions
- ◆ **Report16** -- Surface Tension and pore filling time over salt conc.
- ◆ **Report17** -- Percent pore length filled over time
- ◆ **Report18** -- Ligand-wise cation desolvation energy and time
- ◆ **Report19** -- Ligand-wise cation desolvation energy and time (accounting for CS)
- ◆ **Report20** -- Terms relating to structure and Communal Ion Solvation (CS)

Other than the output report files, the AEM GUI generates two more output files described below.

- **settings-AEM Run Identifier-YYYYMMDD\_hhmmss.json:** This **setting .json** file saves the user's current run settings, which allows user to import them in the future if they want to rerun the same or make small changes to the imported run. This file also is the backbone of the GUI to populate the settings pane in the output page, allowing users a quick glance of the settings for the currently selected run folder.
- **verbose-AEM Run Identifier-YYYYMMDD\_hhmmss.txt:** This **verbose .txt** file is just a more readable version of the values being sent to the AEM command line executables.

In this section, the GUI provides a drop down select option for the user to choose what output report to view. The report chosen is displayed in the **REPORT TEXT** section described in Section 3.4.4, given that the **Text** option is selected in the **Data Display** section described in Section 3.4.3.

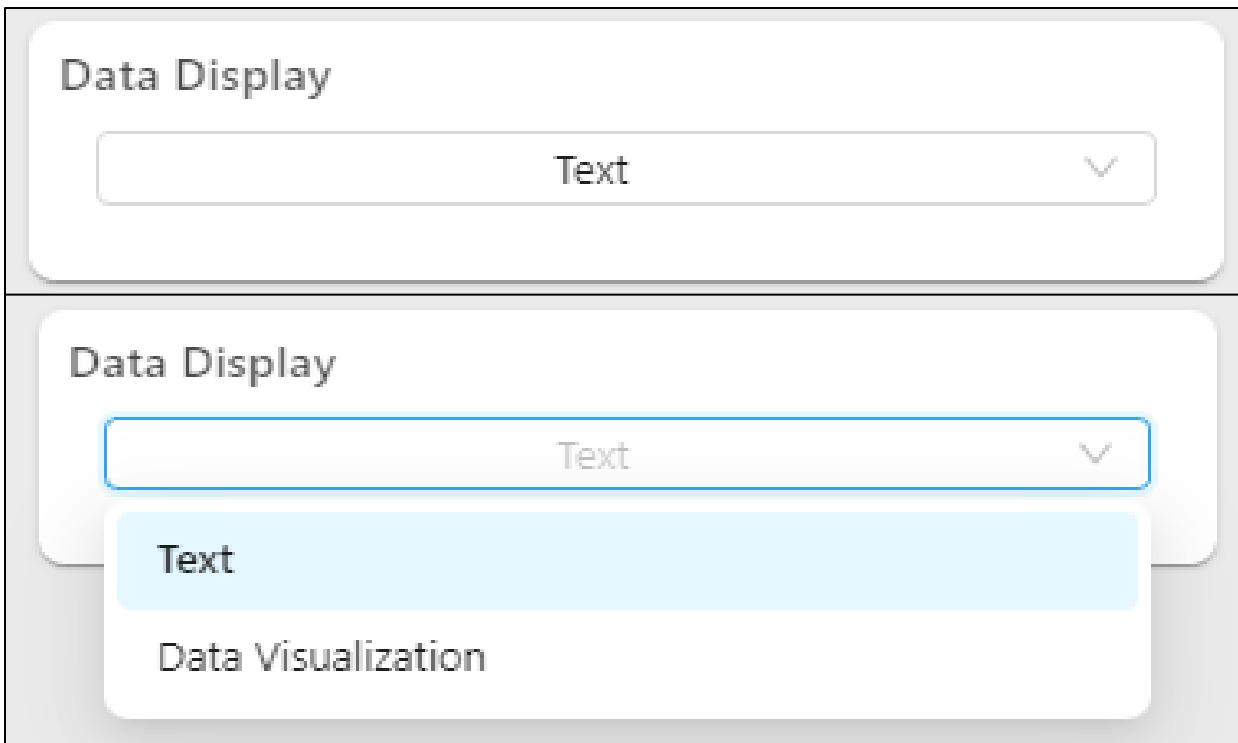
The user can use the **Delete** button (>Delete) to delete the instance for a particular output report file and the **Open in System Editor** button (>Edit) to open the output report file in the default text editor on the user's local machine. A visual of this section is shown in Figure 53 below.



**Figure 53. AEM REPORTS section of the AEM Output tab.**

### **3.4.3 Data Display**

This is a dropdown select option where the user can select whether the output files must be viewed in text format or be plotted and viewed as a graphical representation. The user has two options – **Text** that opens the **REPORT TEXT** section and **Data Visualization** that opens the **REPORT DATA VISUALIZATION** section. A visual of this section is shown in Figure 54 below.



**Figure 54. Data Display section of the AEM Output tab.**

### 3.4.4 REPORT TEXT

This is the section where the user can view any report in **Report01 – Report20**, along with the **settings .json** and **verbose .txt** files using the GUI's inbuilt text viewer scroll box given that the user selects the **Text** option in the **Display Data** section. A visual of the **AEM Output Tab** with the **REPORT TEXT** section for viewing the **Report01 – Report20 Output Report** files (Figure 55), the **settings .json** file (Figure 56), and the **verbose .txt** file (Figure 57) is shown below.

REPORT TEXT

AEM ver. 2.23.1M  
\*\*\* CALCULATIONS ARE PERFORMED ACCOUNTING FOR THE EFFECT OF ION ASSOC. ON HSA PARAMETERS AND OTHER QUANTITIES.

Number of Mixed-Salt Mole Fraction Cases = 1  
k<sub>1</sub>,k<sub>2</sub>,k<sub>3</sub>,k<sub>4</sub>,ksum = 1 0 0 0 1

Results for salt = LiPF<sub>6</sub> at Temp. = -40.00 C or -40.00 F, and 1/T(K) = 0.004289

Solvent composition (salt-free):

Name	Mole Fraction	Mass Fraction	Volume Fraction
ethylene carbonate	0.31985	0.30737	0.25315
dimethyl carbonate	0.49743	0.48899	0.49993
ethyl propionate	0.18271	0.20364	0.24692

Rational Properties:

m <sub>2</sub>	c <sub>2</sub>	wt fr salt	mole fr salt	density (g/cc)	visc. (cP)	sig1 (#efr)	sig2 (#efr)	S(=)	Rational	Diff.	Spec.	
									Act.Coeff.	Coeff.	Cond.	
									cm <sup>-2</sup> /s	y(=)	(m <sup>2</sup> /cm)	
									t <sub>a</sub> (s)	t <sub>b</sub> (s)	dispc	
									t <sub>a</sub> (s)	t <sub>b</sub> (s)	dispc	
0.025	0.029	0.004	0.002	1.160	3.98	8.151	7.131	3.945	0.589E+00	0.299E+00	0.380	0.99999 0.00000
0.050	0.058	0.008	0.005	1.163	4.13	8.146	7.129	3.951	0.522E+00	0.288E+00	0.382	0.99998 0.00000
0.100	0.115	0.015	0.009	1.168	4.46	8.139	7.126	3.969	0.460E+00	0.266E+00	0.385	0.99995 0.00000
0.150	0.174	0.022	0.014	1.172	4.84	8.131	7.122	3.980	0.400E+00	0.244E+00	0.388	0.99992 0.00000
0.200	0.233	0.030	0.020	1.177	5.18	8.123	7.118	3.987	0.342E+00	0.223E+00	0.391	0.99987 0.00001
0.250	0.285	0.037	0.022	1.182	5.57	8.114	7.112	4.009	0.242E+00	0.211E+00	0.395	0.99981 0.00001
0.300	0.340	0.044	0.027	1.187	5.98	8.105	7.106	4.020	0.197E+00	0.156E+01	0.398	0.99973 0.00002
0.350	0.390	0.050	0.031	1.191	6.42	8.096	7.099	4.030	0.1438E+00	0.182E+00	0.172E+01	0.401 0.99964 0.00004
0.400	0.451	0.057	0.035	1.196	6.90	8.086	7.092	4.039	0.1070E+00	0.1707E+01	0.403	0.403 0.99953 0.00005
0.450	0.512	0.064	0.040	1.200	7.45	8.076	7.085	4.048	0.740E+00	0.1694E+01	0.405	0.405 0.99951 0.00005
0.500	0.560	0.071	0.044	1.205	7.96	8.066	7.077	4.049	0.502E+00	0.1476E+00	0.409	0.409 0.99922 0.00014
0.550	0.614	0.077	0.044	1.210	8.56	8.055	7.069	4.053	0.534E+00	0.136E+01	0.412	0.412 0.99900 0.00020
0.600	0.664	0.084	0.052	1.214	9.22	8.045	7.061	4.054	0.573E+00	0.127E+00	0.415	0.415 0.99874 0.00029
0.650	0.721	0.099	0.056	1.219	9.94	8.034	7.051	4.055	0.618E+00	0.117E+00	0.418	0.418 0.99842 0.00042
0.700	0.777	0.112	0.061	1.223	10.63	8.013	7.034	4.056	0.662E+00	0.107E+00	0.421	0.421 0.99809 0.00049
0.750	0.826	0.102	0.064	1.228	11.63	8.013	7.024	4.051	0.736E+00	0.100E+00	0.424	0.424 0.99764 0.00089
0.800	0.879	0.108	0.068	1.232	12.63	8.003	7.014	4.046	0.811E+00	0.925E+00	0.427	0.427 0.99720 0.00107
0.850	0.931	0.114	0.072	1.236	13.74	7.992	7.015	4.040	0.899E+00	0.850E+00	0.429	0.429 0.99666 0.00143
0.900	0.982	0.120	0.076	1.241	14.98	7.981	7.005	4.032	0.100E+01	0.780E+00	0.432	0.432 0.99597 0.00191
0.950	1.034	0.126	0.080	1.245	16.39	7.971	6.996	4.012	0.112E+01	0.714E+00	0.435	0.435 0.99511 0.00254
1.000	1.085	0.132	0.084	1.249	17.99	7.960	6.986	4.000	0.126E+01	0.651E+00	0.438	0.438 0.99402 0.00338
1.050	1.135	0.138	0.088	1.254	19.79	7.950	6.976	3.987	0.143E+01	0.592E+00	0.440	0.440 0.99267 0.00445

Figure 55. REPORT TEXT section of the AEM Output tab – Viewing the Report01 – Report20 Output Report files.

REPORT TEXT

Example 1-20230516\_113901\settings-Example 1-20230516\_113901.json

```
{
  "mode": 1,
  "volumeMass": 1,
  "fixedArr": [
    {
      "volume": "25",
      "error": 0,
      "solvent": [
        -6,
        -12
      ]
    },
    {
      "volume": "50",
      "error": 0,
      "solvent": [
        -1,
        -8
      ]
    },
    {
      "volume": "25",
      "error": 0,
      "solvent": [
        -1,
        -3
      ]
    }
  ],
  "matrixArr": [
    {
      "constmassfrac": "",
      "cfcb": false,
      "error": false
    }
  ],
  "saltMode": 1,
  "saltArr": [
    {
      "salt": [
        1,
        2,
        3
      ],
      "molar": "",
      "error": false
    }
  ],
  "saltConc": "5",
  "tMin": "-30"
}
```

Figure 56. REPORT TEXT section of the AEM Output tab – Viewing the settings.json file.

```

REPORT TEXT
Example 1-20230516_113901verbose-Example 1-20230516_113901.txt

SINGLE FIXED COMPOSITION OF SOLVENTS: 1
OPTION (1)Volume or (2) MASS: 1
NUMBER OF SOLVENTS: 3
Input Number for Solvent 1 : 12
Input Number for Solvent 2 : 8
Input Number for Solvent 3 : 3
Input Percent for Solvent 1 : 25
Input Percent for Solvent 2 : 50
Input Percent for Solvent 3 : 25
NUMBER OF salts: 1
Input Number for Solvent 1 : 7
Salt Conc: 5
TMIN: 30
TMAX: 60
TSTEP: 5
ION STABILITY: 1
CONTACT ANGLE: 35
PORE DIAMETER: 20
SALT CONCENTRATION OF INTEREST: 1.5
USE SCAEP: 0
USE DOUBLE LAYER: 0

```

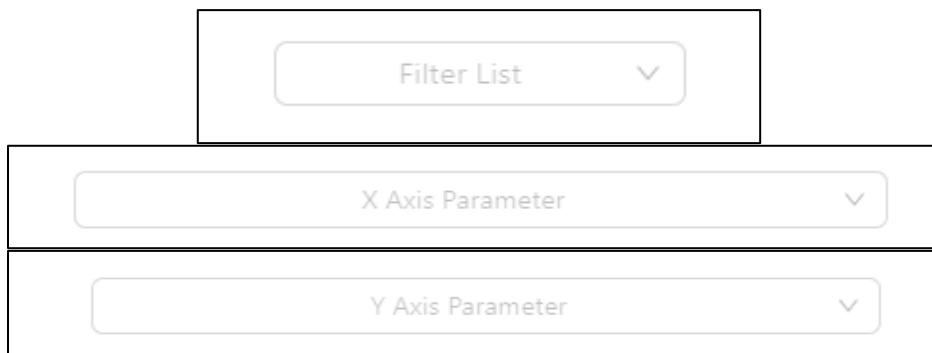
**Figure 57. REPORT TEXT section of the AEM Output tab – Viewing the verbose .txt file.**

### 3.4.5 REPORT DATA VISUALIZATION

This is the section where the user can plot the output parameters from **Report01 – Report20** using the GUI's built-in graphing capability. This functionality is enabled when the user selects the Data Visualization option. The output parameters for each output report are defined in detail in Section 7.1.1. The GUI provides the user with the following three drop down sections.

- **Filter List** - This is a drop down select option to filter the parameters being plotted based on Temperature, Salt Composition, and Solvent Composition.
- **X-Axis Parameter & Y-Axis Parameter** - These are drop down select options to plot various output parameters on the X-Axis and Y-Axis.

A visual of the three drop down select options (Figure 58) and the entire **AEM Output** Tab with the **REPORT DATA VISUALIZATION** section (Figure 59) is shown in the following Figures. Also note that individual results from certain data output reports can be exported to a .csv file using the export button under the Temperature ID. This functionality allows for easy export and use into other software programs for further analysis and visualization.



**Figure 58. REPORT DATA VISUALIZATION section of the AEM Output tab – 3 select drop down options.**

## Advanced Electrolyte Model (AEM)

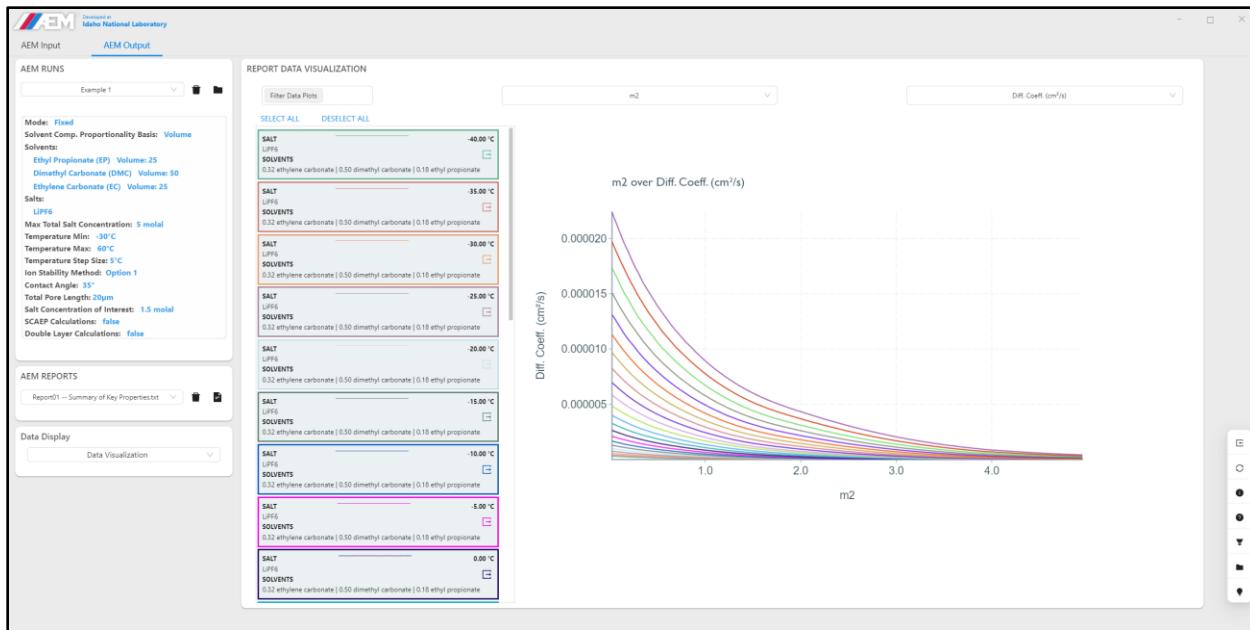


Figure 59. REPORT DATA VISUALIZATION section of the AEM Output tab.

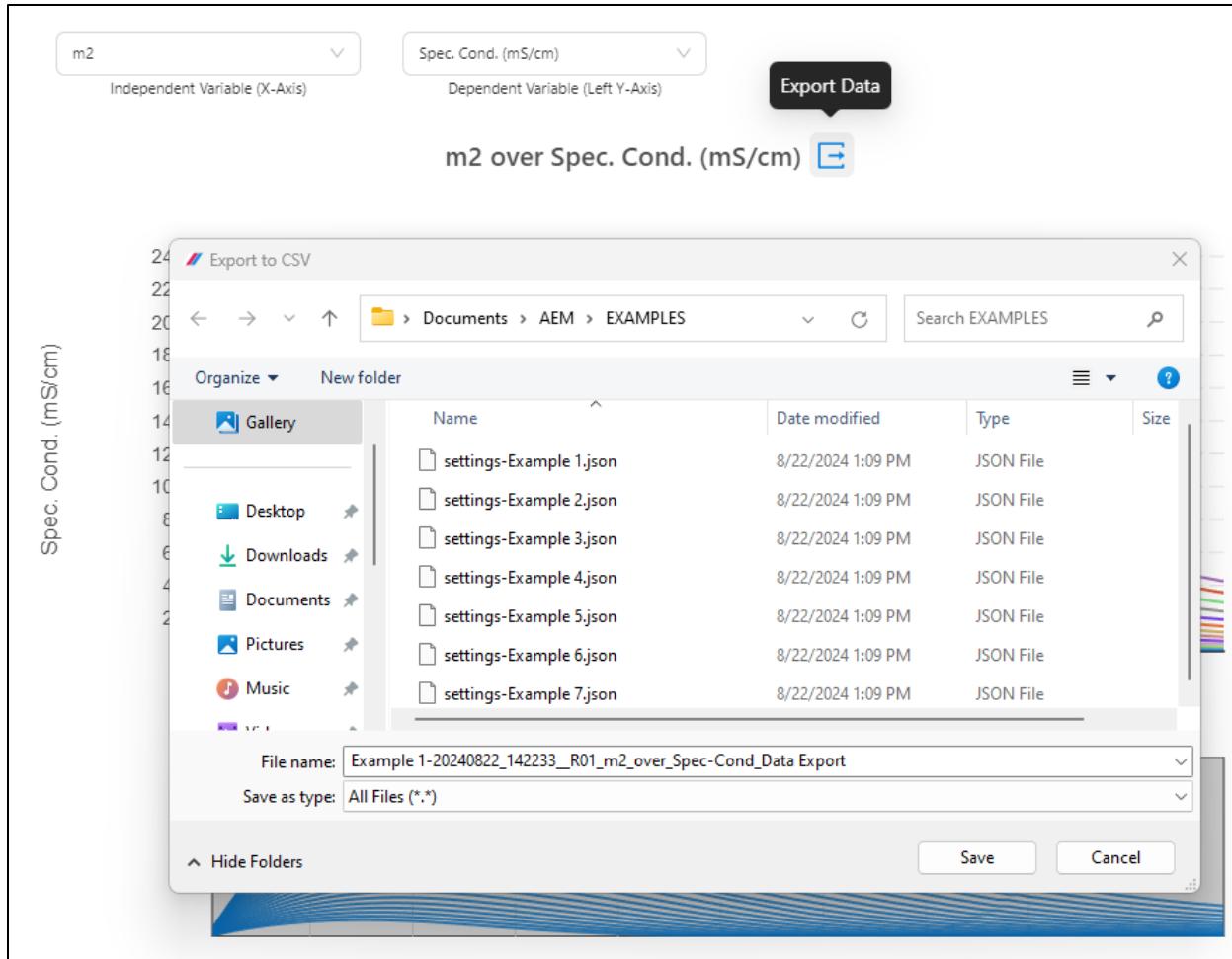
**Important Note:** Not all generated data output in Report01 – Report20 have plotting and export to .csv capabilities. In such cases, only the text data output is displayed. The AEM GUI also has a built-in limit to only parse and display data output reports that are less than 500 MB.

### 3.4.6 REPORT DATA EXTRACTION

This is the section where the user can extract the output parameters from **Report01 – Report20** using the GUI's built-in graphing capability. This functionality is enabled when the user selects the Data Visualization option and then has a choice to either export data for a single parameter or all parameters for a particular report into a single CSV file. This feature would help users to extract meaningful data for external analysis. The two options are further described below with appropriate visualizations:

- **Single Parameter Export:** Users can export any parameter values for a particular report for either all temperatures or a range of temperatures to a csv file. The blue icon beside the figure title as shown in Figure 60, pops up a window that enables the user to save the file at a user specified location. The user can either choose the default name or can specify their own and hit on the "Save" button. A snapshot for the layout of the csv extracted for this feature is shown in Figure 61. The first column represents the X axis and represents the parameter as chosen in the GUI before exporting the file. The other columns represent the values of the parameter of interest for all range of temperature selected during export. This capability helps users for external analysis.

## Advanced Electrolyte Model (AEM)



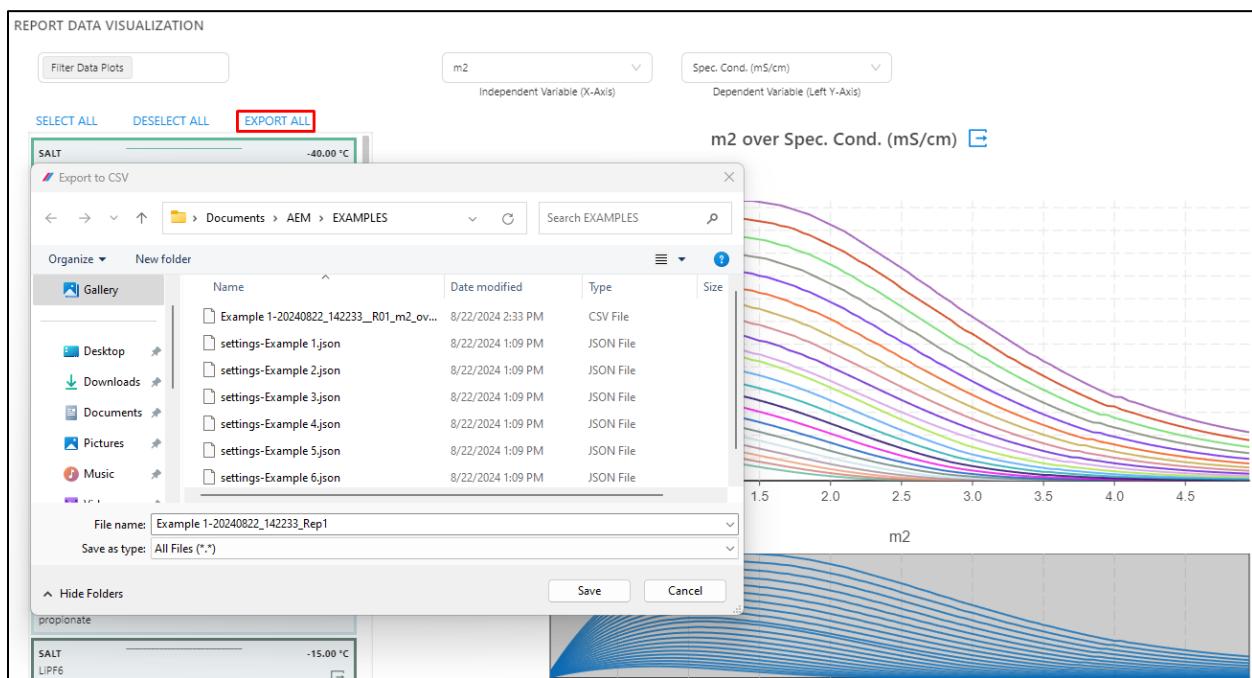
**Figure 60. Single Parameter Export Feature**

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	m2	-40.00C	Li-35.00C	Li-30.00C	Li-25.00C	Li-20.00C	Li-15.00C	Li-10.00C	Li-5.00C	Li@0.00C	Li@5.00C	Li@10.00C	Li@15.00C	Li@20.00C	Li@25.00C	Li@30.00C	Li@35.00C	Li@40.00C	Li@45.00C	Li@50.00C	Li@55.00C
2	0.025	0.173	0.202	0.232	0.265	0.3	0.337	0.376	0.417	0.46	0.505	0.551	0.599	0.647	0.698	0.749	0.801	0.854	0.908	0.962	1.02
3	0.05	0.338	0.393	0.453	0.518	0.586	0.659	0.737	0.817	0.902	0.99	1.08	1.17	1.27	1.37	1.47	1.57	1.68	1.78	1.89	2

 The data continues with more rows of numerical values, indicating a large dataset being exported."/>

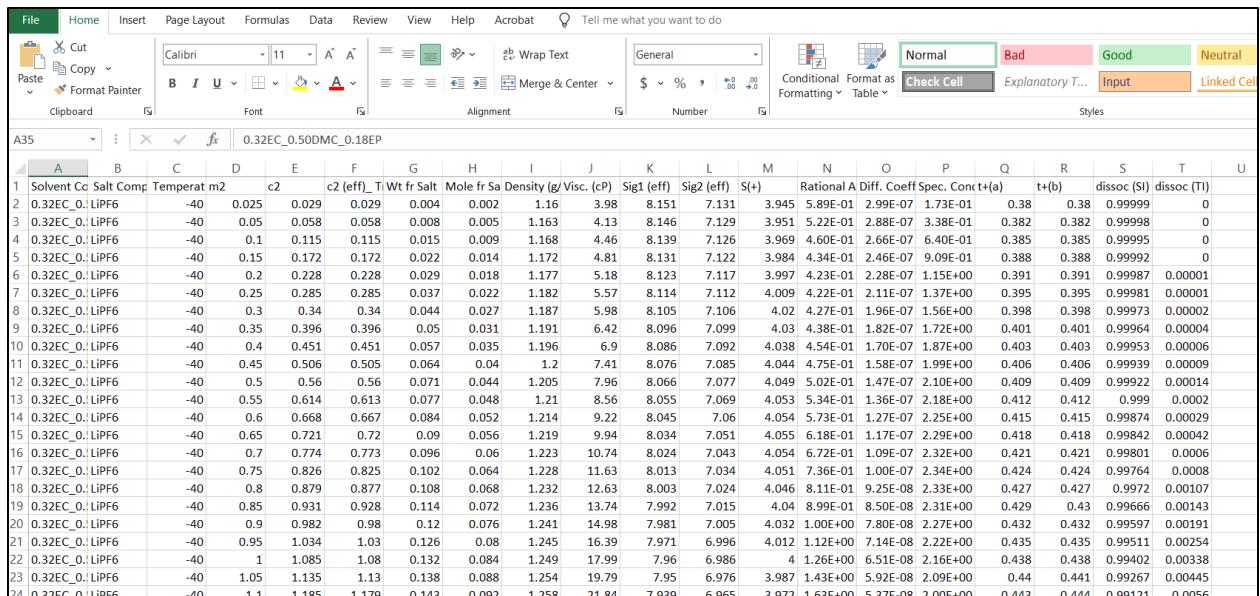
**Figure 61. Layout for the csv exported for a single parameter**

- **EXPORT ALL Feature:** Users can export the entire report containing all the parameters for all temperatures in to a csv file. The blue icon "EXPORT ALL" highlighted in **red rectangle** as shown in Figure 62, pops up a window that enables the user to save the file at a user specified location. The user can either choose the default name or can specify their own and hit on the "Save" button. A snapshot for the layout of the csv extracted for this feature is shown in Figure 63. The first column represents the solvent composition, the second column represents the salt composition, the third column represents the temperatures and the rest of the columns are for all the properties for a certain report. This capability can be reproduced for all other reports as well. This capability helps users for external analysis.



**Figure 62. EXPORT ALL Feature**

## Advanced Electrolyte Model (AEM)



	Solvent	Cc	Salt Comp	Temperat	m2	c2	c2 (eff)	Ti	Wt fr Salt	Mole fr Sa	Density (g/Visc.	(c.P.)	Sig1 (eff)	Sig2 (eff)	S(t)	Rational	Diff. Coeff Spec.	Cont (t+a)	t+(b)	dissoc (SI)	dissoc (TI)
1	Solvent	Cc	Salt Comp	Temperat	m2	c2	c2 (eff)	Ti	Wt fr Salt	Mole fr Sa	Density (g/Visc.	(c.P.)	Sig1 (eff)	Sig2 (eff)	S(t)	Rational	Diff. Coeff Spec.	Cont (t+a)	t+(b)	dissoc (SI)	dissoc (TI)
2	0.32EC_0.:LiPF6	-40	0.025	0.029	0.029	0.004	0.002	1.16	3.98	8.151	7.131	3.945	5.89E-01	2.99E-07	1.73E-01	0.38	0.38	0.99999	0		
3	0.32EC_0.:LiPF6	-40	0.05	0.058	0.058	0.008	0.005	1.163	4.13	8.146	7.129	3.951	5.22E-01	2.88E-07	3.38E-01	0.382	0.382	0.99998	0		
4	0.32EC_0.:LiPF6	-40	0.1	0.115	0.115	0.015	0.009	1.168	4.46	8.139	7.126	3.969	4.60E-01	2.66E-07	6.40E-01	0.385	0.385	0.99995	0		
5	0.32EC_0.:LiPF6	-40	0.15	0.172	0.172	0.022	0.014	1.172	4.81	8.131	7.122	3.984	4.34E-01	2.46E-07	9.09E-01	0.388	0.388	0.99992	0		
6	0.32EC_0.:LiPF6	-40	0.2	0.228	0.228	0.029	0.018	1.177	5.18	8.123	7.117	3.997	4.23E-01	2.28E-07	1.15E+00	0.391	0.391	0.99987	0.00001		
7	0.32EC_0.:LiPF6	-40	0.25	0.285	0.285	0.037	0.022	1.182	5.57	8.114	7.112	4.009	4.22E-01	2.11E-07	1.37E+00	0.395	0.395	0.99981	0.00001		
8	0.32EC_0.:LiPF6	-40	0.3	0.34	0.34	0.044	0.027	1.187	5.98	8.105	7.106	4.02	4.27E-01	1.96E-07	1.56E+00	0.398	0.398	0.99973	0.00002		
9	0.32EC_0.:LiPF6	-40	0.35	0.396	0.396	0.05	0.031	1.191	6.42	8.09	7.099	4.03	4.38E-01	1.82E-07	1.72E+00	0.401	0.401	0.99964	0.00004		
10	0.32EC_0.:LiPF6	-40	0.4	0.451	0.451	0.057	0.035	1.196	6.9	8.086	7.092	4.038	4.54E-01	1.70E-07	1.87E+00	0.403	0.403	0.99953	0.00006		
11	0.32EC_0.:LiPF6	-40	0.45	0.506	0.505	0.064	0.04	1.2	7.41	8.076	7.085	4.044	4.75E-01	1.58E-07	1.99E+00	0.406	0.406	0.99939	0.00009		
12	0.32EC_0.:LiPF6	-40	0.5	0.56	0.56	0.071	0.044	1.205	7.96	8.066	7.077	4.049	5.02E-01	1.47E-07	2.10E+00	0.409	0.409	0.99922	0.00014		
13	0.32EC_0.:LiPF6	-40	0.55	0.614	0.613	0.077	0.048	1.21	8.56	8.055	7.069	4.053	5.34E-01	1.36E-07	2.18E+00	0.412	0.412	0.999	0.0002		
14	0.32EC_0.:LiPF6	-40	0.6	0.668	0.667	0.084	0.052	1.214	9.22	8.045	7.06	4.054	5.73E-01	1.27E-07	2.25E+00	0.415	0.415	0.99874	0.00029		
15	0.32EC_0.:LiPF6	-40	0.65	0.721	0.72	0.09	0.056	1.219	9.94	8.034	7.051	4.055	6.18E-01	1.17E-07	2.29E+00	0.418	0.418	0.99842	0.00042		
16	0.32EC_0.:LiPF6	-40	0.7	0.774	0.773	0.096	0.06	1.223	10.74	8.024	7.043	4.054	6.72E-01	1.09E-07	2.32E+00	0.421	0.421	0.99801	0.0006		
17	0.32EC_0.:LiPF6	-40	0.75	0.826	0.825	0.102	0.064	1.228	11.63	8.013	7.034	4.051	7.36E-01	1.00E-07	2.34E+00	0.424	0.424	0.99764	0.0008		
18	0.32EC_0.:LiPF6	-40	0.8	0.879	0.877	0.108	0.068	1.232	12.63	8.003	7.024	4.046	8.11E-01	9.25E-08	2.33E+00	0.427	0.427	0.9972	0.00107		
19	0.32EC_0.:LiPF6	-40	0.85	0.931	0.928	0.114	0.072	1.236	13.74	7.992	7.015	4.04	8.99E-01	8.50E-08	2.31E+00	0.429	0.43	0.99666	0.00143		
20	0.32EC_0.:LiPF6	-40	0.9	0.982	0.98	0.12	0.076	1.241	14.98	7.981	7.005	4.032	1.00E+00	7.80E-08	2.27E+00	0.432	0.432	0.99597	0.00191		
21	0.32EC_0.:LiPF6	-40	0.95	1.034	1.03	0.126	0.08	1.245	16.39	7.971	6.996	4.012	1.12E+00	7.14E-08	2.22E+00	0.435	0.435	0.99511	0.00254		
22	0.32EC_0.:LiPF6	-40	1	1.085	1.08	0.132	0.084	1.249	17.99	7.96	6.986	4	1.26E+00	6.51E-08	2.16E+00	0.438	0.438	0.99402	0.00338		
23	0.32EC_0.:LiPF6	-40	1.05	1.135	1.13	0.138	0.088	1.254	19.79	7.95	6.976	3.987	1.43E+00	5.92E-08	2.09E+00	0.44	0.441	0.99267	0.00445		
24	0.32EC_0.:LiPF6	-40	1.1	1.185	1.179	0.142	0.092	1.258	21.84	7.020	6.065	3.072	1.63E+00	5.37E-08	2.00E+00	0.442	0.444	0.99121			

**Figure 63.** Layout for the csv exported for EXPORT ALL feature

## 3.5 Global Features & Icons

There are seven (7) primary operating buttons that can be considered as global features. The program also supports a global input that is used to save a list of all defined simulation conditions in a unique json file, that can be stored for future use. A brief overview of each global feature is outlined below:

- Import Button:** This button allows a user to import a full set of simulation conditions from a .json file that is stored in the **C:\Users\user-name\Documents\AEM\EXAMPLES\** subdirectory. When selected, this button will open a Windows File Explorer for the user to search for a .json file from a particular simulation for the inputs defined by the user. This feature is very useful when trying to rerun previous AEM simulations as well as existing examples covered in the User Guide. After a .json file is selected for import, the program will prepopulate all simulation conditions to be specified in each tab.



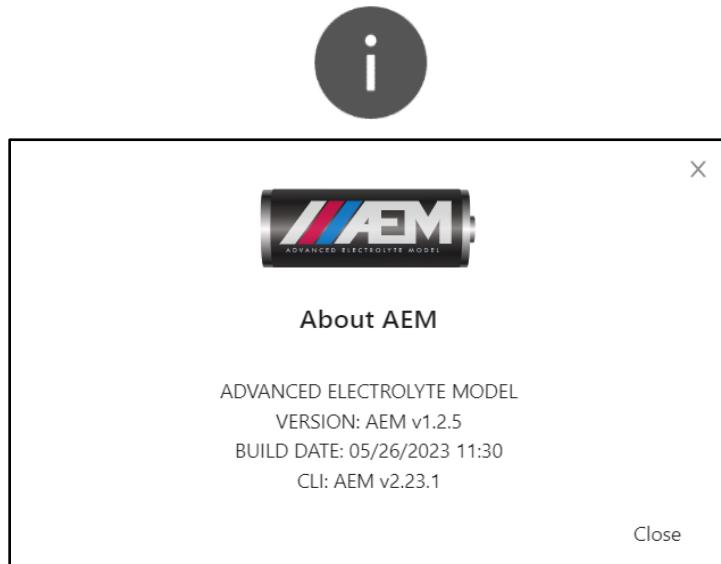
**Figure 64.** Icon for GUI Import Button.

- Reset Inputs Button:** This button can be pressed to start a new simulation from scratch. It will clear all the initial inputs supplied by the user and reset the AEM GUI to start over.



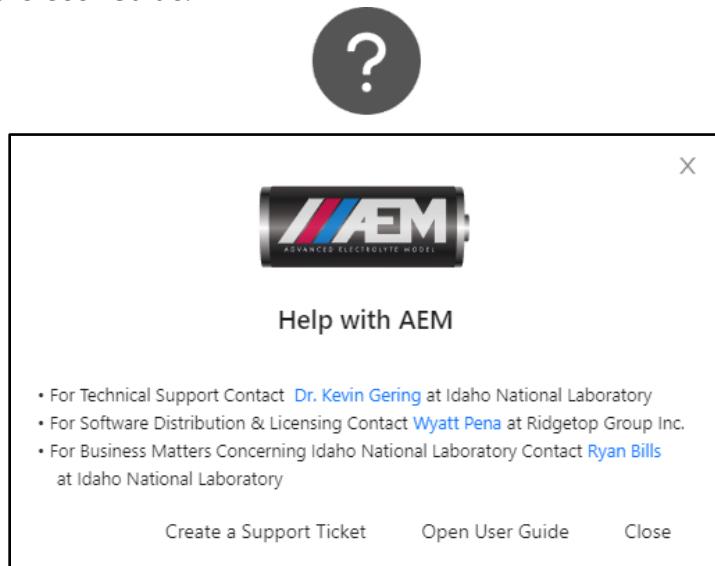
**Figure 65. Icon for GUI Reset Inputs Button.**

3. **Information Button:** This button will generate a pop-up window and tell the user what version of the GUI they are working with.



**Figure 66. Icon and pop-up message for GUI Information Button.**

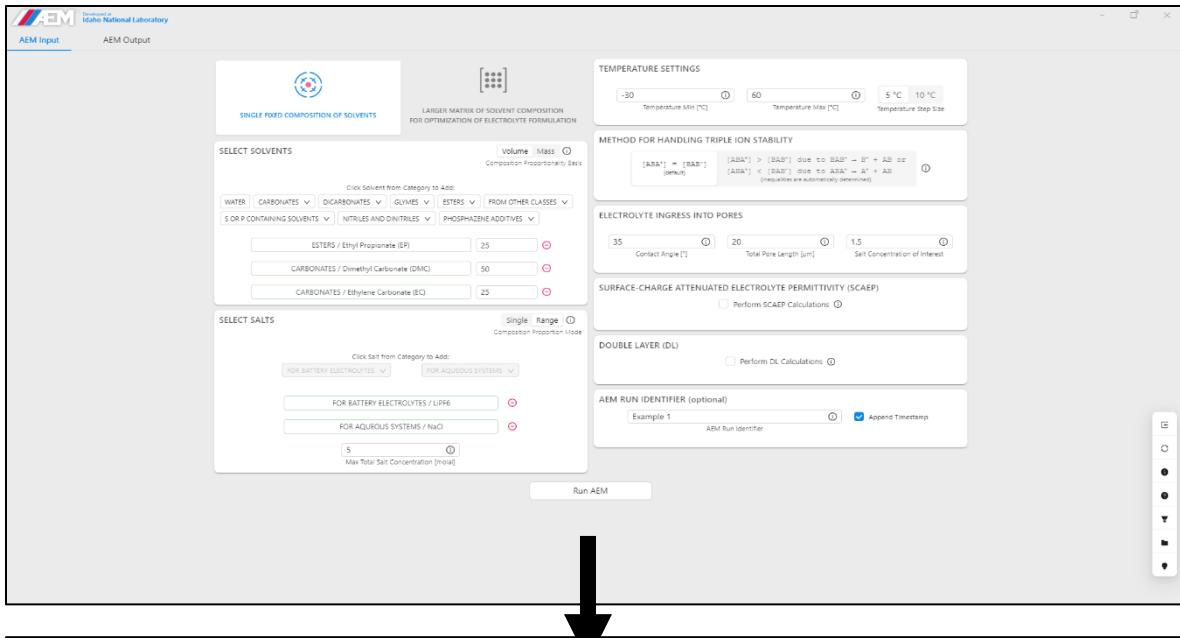
4. **Help Button:** This button will open a pop-up window with hyperlinks to create a Support Ticket and open the User Guide.



**Figure 67. Icon and pop-up message for GUI Help Button.**

5. **Expanded / Compact Format Button:** This button will change the format of the AEM GUI to an expanded or compact view when selecting Solvents and Salts.

## Advanced Electrolyte Model (AEM)



**AEM Input**      **AEM Output**

**SINGLE FIXED COMPOSITION OF SOLVENTS**

**LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION**

**SELECT SOLVENTS**

Volume Mass Composition Proportion (molar)

Click Solvent from Category to Add:

- WATER
- CARBONATES
- DICARBOLENES
- GLYCOMES
- ESTERS
- FROM OTHER CLASSES
- S OR P CONTAINING SOLVENTS
- NITRILES AND DINITRILES
- PHOSPHAZENE ADDITIVES

ESTERS / Ethyl Propionate (EP) 25

CARBONATES / Dimethyl Carbonate (DMC) 50

CARBONATES / Ethylene Carbonate (EC) 25

**SELECT SALTS**

Single Range Composition Proportion (molar)

Click Salt from Category to Add:

- FOR BATTERY ELECTROLYTES / LiPF6
- FOR AQUEOUS SYSTEMS / NaCl

LiPF6 5

Max Total Salt Concentration (molar)

**TEMPERATURE SETTINGS**

Temperature Min [°C] 30    Temperature Max [°C] 60    Temperature Step Size 5 °C    10 °C

**METHOD FOR HANDLING TRIPLE ION STABILITY**

[ $\text{[A}^{\pm}\text{]} = \text{[B}^{\pm}\text{]}$ ]    [ $\text{[A}^{\pm}\text{]} > \text{[B}^{\pm}\text{]}$ ] due to  $\text{[A}^{\pm}\text{]} = \text{B}^{\pm} + \text{AB}$  or  
[ $\text{[A}^{\pm}\text{]} < \text{[B}^{\pm}\text{]}$ ] due to  $\text{[A}^{\pm}\text{]} = \text{A}^{\pm} + \text{AB}$   
(inequalities are automatically determined)

**ELECTROLYTE INGRESS INTO PORES**

Contact Angle [°] 35    Total Pore Length [μm] 20    Salt Concentration of Interest 1.5

**SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**

Perform SCAEP Calculations

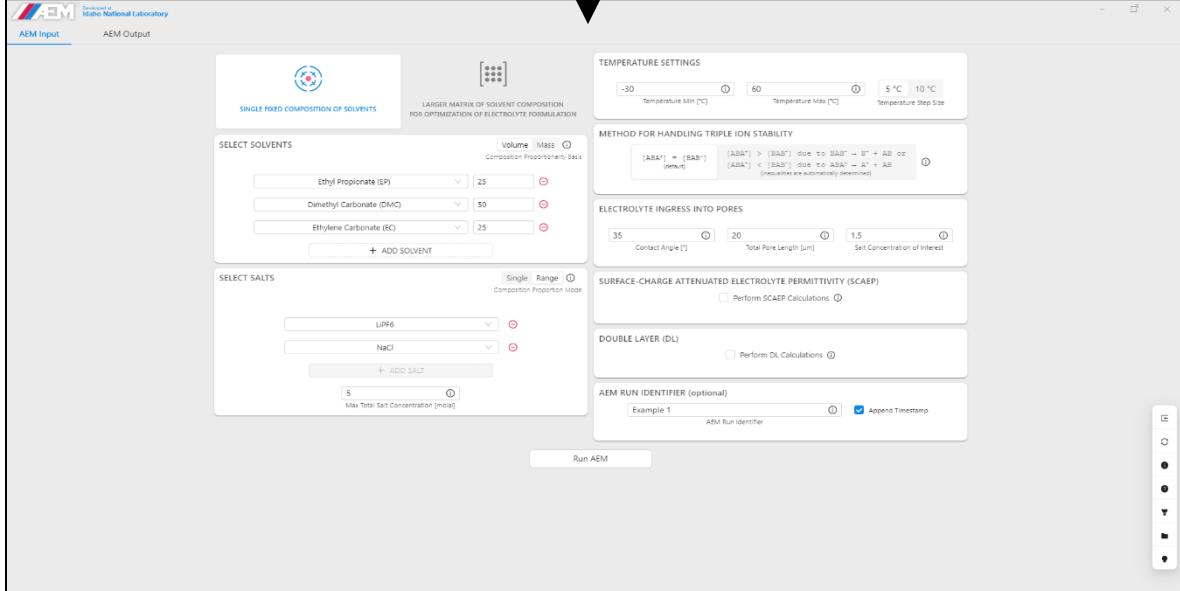
**DOUBLE LAYER (DL)**

Perform DL Calculations

**AIM RUN IDENTIFIER (optional)**

Example 1    AIM Run Identifier     Append Timestamp

Run AEM



**AEM Input**      **AEM Output**

**SINGLE FIXED COMPOSITION OF SOLVENTS**

**LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION**

**SELECT SOLVENTS**

Volume Mass Composition Proportion (molar)

Ethyl Propionate (EP) 25

Dimethyl Carbonate (DMC) 50

Ethylene Carbonate (EC) 25

+ ADD SOLVENT

**SELECT SALTS**

Single Range Composition Proportion (molar)

LiPF6 5

NaCl 0

+ ADD SALT

S 5

Max Total Salt Concentration (molar)

**TEMPERATURE SETTINGS**

Temperature Min [°C] 30    Temperature Max [°C] 60    Temperature Step Size 5 °C    10 °C

**METHOD FOR HANDLING TRIPLE ION STABILITY**

[ $\text{[A}^{\pm}\text{]} = \text{[B}^{\pm}\text{]}$ ]    [ $\text{[A}^{\pm}\text{]} > \text{[B}^{\pm}\text{]}$ ] due to  $\text{[A}^{\pm}\text{]} = \text{B}^{\pm} + \text{AB}$  or  
[ $\text{[A}^{\pm}\text{]} < \text{[B}^{\pm}\text{]}$ ] due to  $\text{[A}^{\pm}\text{]} = \text{A}^{\pm} + \text{AB}$   
(inequalities are automatically determined)

**ELECTROLYTE INGRESS INTO PORES**

Contact Angle [°] 35    Total Pore Length [μm] 20    Salt Concentration of Interest 1.5

**SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**

Perform SCAEP Calculations

**DOUBLE LAYER (DL)**

Perform DL Calculations

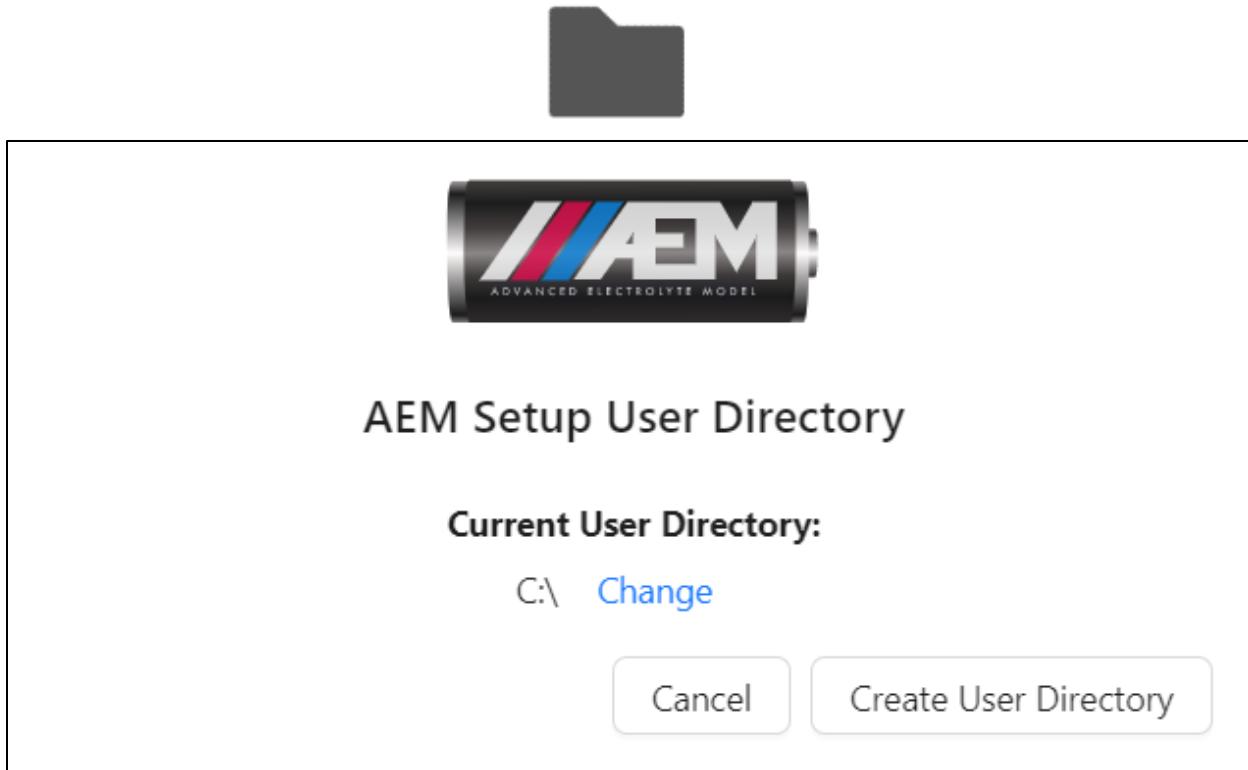
**AIM RUN IDENTIFIER (optional)**

Example 1    AIM Run Identifier     Append Timestamp

Run AEM

**Figure 68. Icon and visual aid for Expanded Format (Top) and Compact Format (Bottom).**

6. **Select New User Directory Button:** This button will open a pop-up window where the user can specify the location for the default folder where the AEM directory needs to be placed.

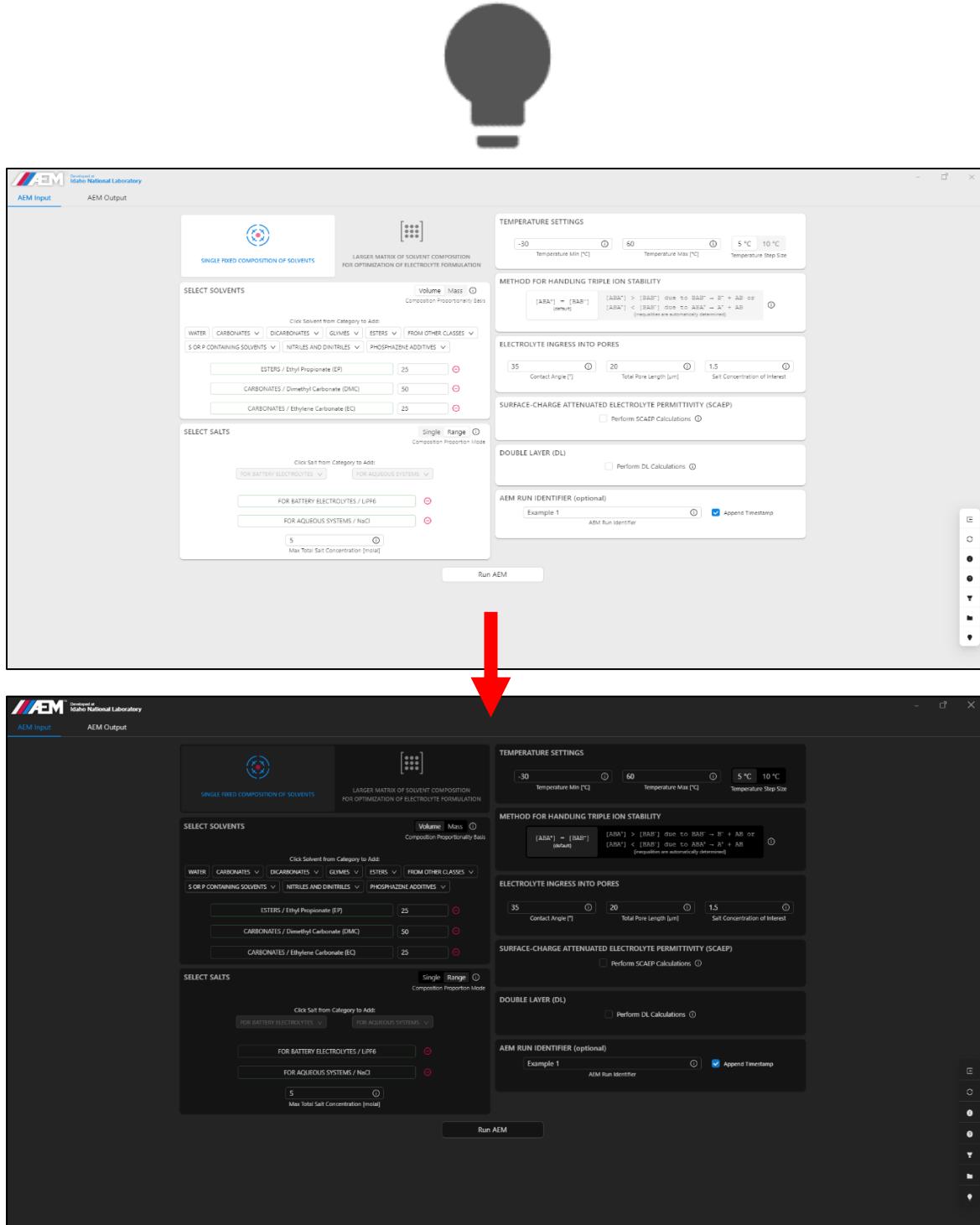


**Figure 69. Icon and pop-up message when changing the default program directory.**

**Important Note:** It is recommended that the AEM folder be inside the **My Documents** or **C:\** directories.

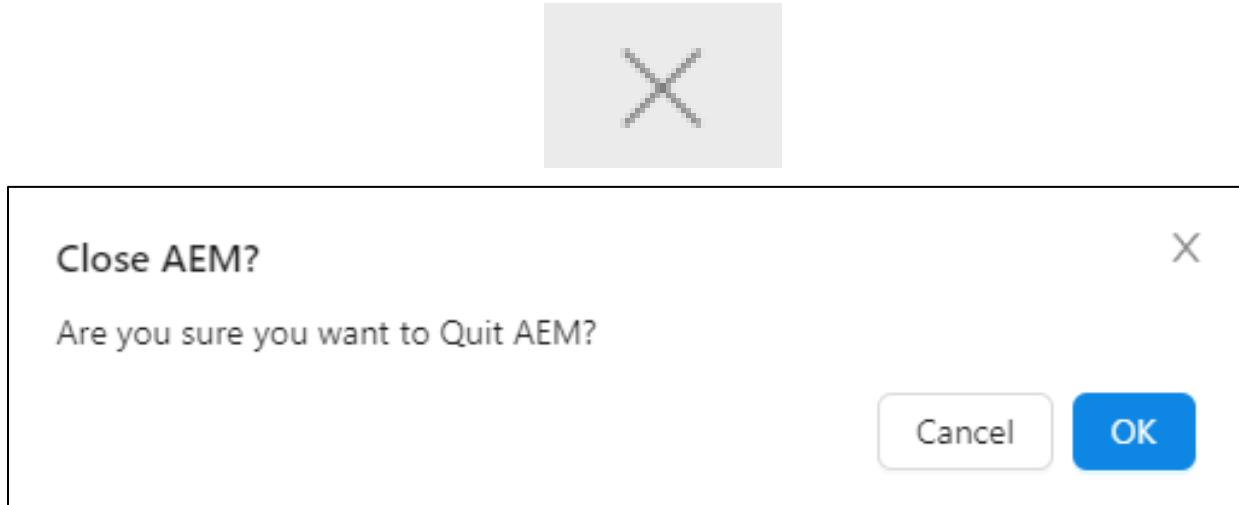
## Advanced Electrolyte Model (AEM)

7. **Dark Mode / Light Mode Toggle Button:** This button can be pressed to switch the AEM GUI to a dark mode. This is ideal for using the AEM GUI at night or in locations where too much stray light is not desired.



**Figure 70. Icon and visual aid for GUI in Light Mode (Top) and Dark Mode (Bottom).**

8. **Exit Button:** This button will prompt the user if they would like to close and exit the program as shown below. The simulation conditions that have been selected will not be remembered, so a user should only exit the program when they wish to close it. If the user selects **OK** the GUI will close and if the user selects **Cancel**, the prompt will close itself.



**Figure 71. Icon and pop-up message for the Exit Button.**

## 4 Examples

Five electrolyte examples are explored herein to provide useful simulation details to the user and to provide context for the selection process. Through this the user can anticipate simulation outcomes for diverse examples ranging from simple to complex, non-aqueous and aqueous.

While AEM is a robust code, please note that not every conceivable input condition or electrolyte combination will be viable within the chemical physics of AEM. Much effort has been devoted to allowing for wide ranges of conditions for temperature, salt concentration and solvent composition, to support an enormous amount of territory to be explored with AEM. Some simple guidance: cases where AEM doesn't run or terminates early are rare, but if the program doesn't run and terminate as expected, this could be due to excessively low temperatures or salt concentrations that are too high. If the code does not terminate as normal in such cases, the Report files often contain output up to the point of termination. To reduce the occurrence of premature termination, try increasing the low temperature limit and/or decreasing the maximum salt concentration.

### 4.1 Example 1: Fixed Volume Proportions for 3-Solvent, 1-Salt System

This example considers the three-solvent system EC, DMC, EP at a fixed volume fraction composition (25, 50, 25 vol %) with LiPF<sub>6</sub>. The salt concentration is allowed to go to 5 molal. Other factors behind the simulation include:

- T = -30°C to 60°C with 5°C steps,
- Used default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal,
- No SCAEP; No DL.

The parameters for electrolyte ingress are relevant estimations for battery electrode materials in general and can be updated to reflect more finely tuned attributes of the porous media.

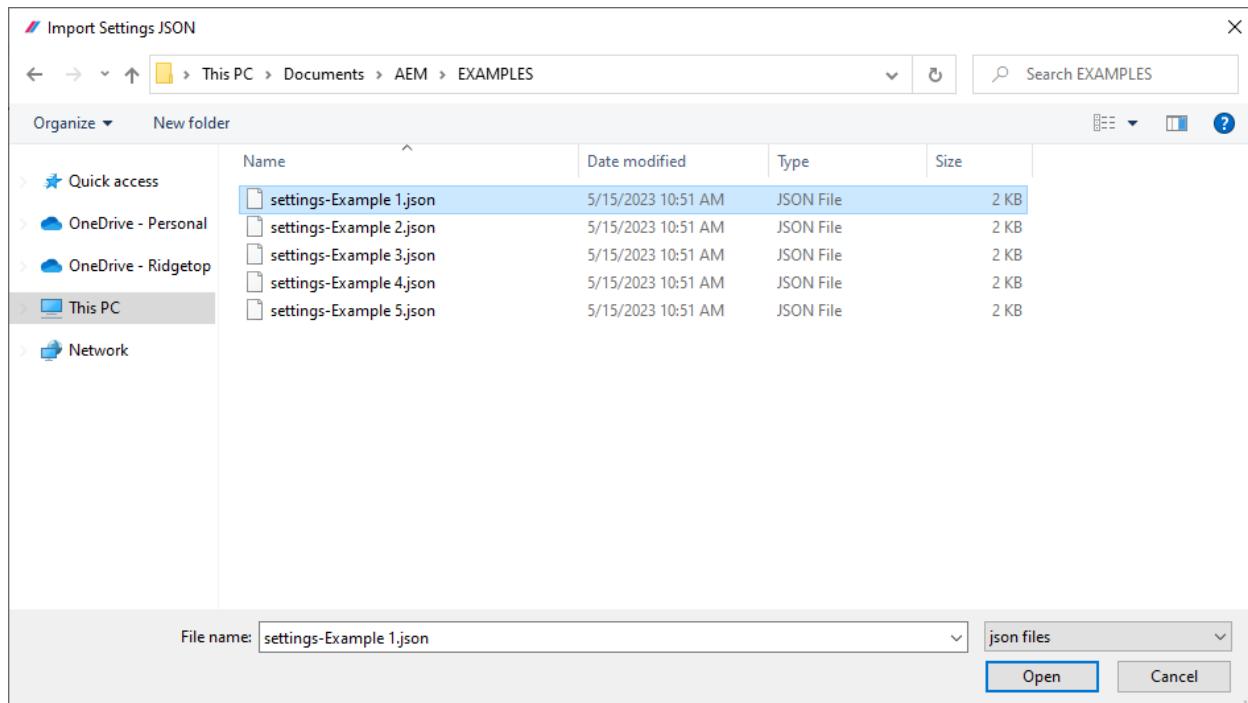
This relatively simple electrolyte represents a lower-viscosity, higher-conductivity system that would facilitate higher current densities in lithium-ion type cells. This electrolyte system has benefits toward conditions like moderately-fast charging and higher-power applications.

#### 4.1.1 Example 1: Importing Example 1 Parameters

We start off Example 1 by first using the **Import** Button from section 3.5 to prepopulate each of the AEM input conditions for Example 1. This can be achieved by following the list of below instructions and referencing Figure 72 and Figure 73.

- a) Click on the **Import** ( ) Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- b) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- c) Select the **settings-Example 1.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 1.json" file was not imported successfully.



**Figure 72. Importing Example 1 Input Condition using the settings-Example 1.json file.**

### 4.1.2 Example 1: Overview of Simulation Input Conditions

Based on the conditions mentioned at the beginning of this example, select the following input conditions:

- EP, DMC, EC at a fixed volume fraction composition (25, 50, 25 vol %)
- LiPF<sub>6</sub> with salt concentration maximum of 5 molal.
- T = -30°C to 60°C with 5°C steps,
- Choose default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35° , Pore length = 20µm, salt conc. of interest = 1.5 molal,
- Choose No SCAEP; No DL.

## Advanced Electrolyte Model (AEM)

The screenshot shows the 'AEM Input' tab with several sections:

- SINGLE FIXED COMPOSITION OF SOLVENTS**: Includes a circular icon with a stylized molecule and a grid icon.
- LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION**: Shows a 4x4 grid icon.
- TEMPERATURE SETTINGS**: Set to -30, 60, 5 °C, 10 °C, and Temperature Step Size.
- METHOD FOR HANDLING TRIPLE ION STABILITY**: Shows inequalities:  $[ABA^+] = [BAB^-]$  (default),  $[ABA^+] > [BAB^-]$  due to  $BAB^- \rightarrow B^+ + AB$ , or  $[ABA^+] < [BAB^-]$  due to  $ABA^+ \rightarrow A^+ + AB$ . It notes that inequalities are automatically determined.
- ELECTROLYTE INGRESS INTO PORES**: Set to Contact Angle 35°, Total Pore Length 20 μm, and Salt Concentration of Interest 1.5 molal.
- SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**: Includes a checkbox for 'Perform SCAEP Calculations'.
- DOUBLE LAYER (DL)**: Includes a checkbox for 'Perform DL Calculations'.
- AEM RUN IDENTIFIER (optional)**: Set to Example 1, with a checked 'Append Timestamp' option.

At the bottom is a 'Run AEM' button.

**Figure 73. Example 1 – AEM Input tab.**

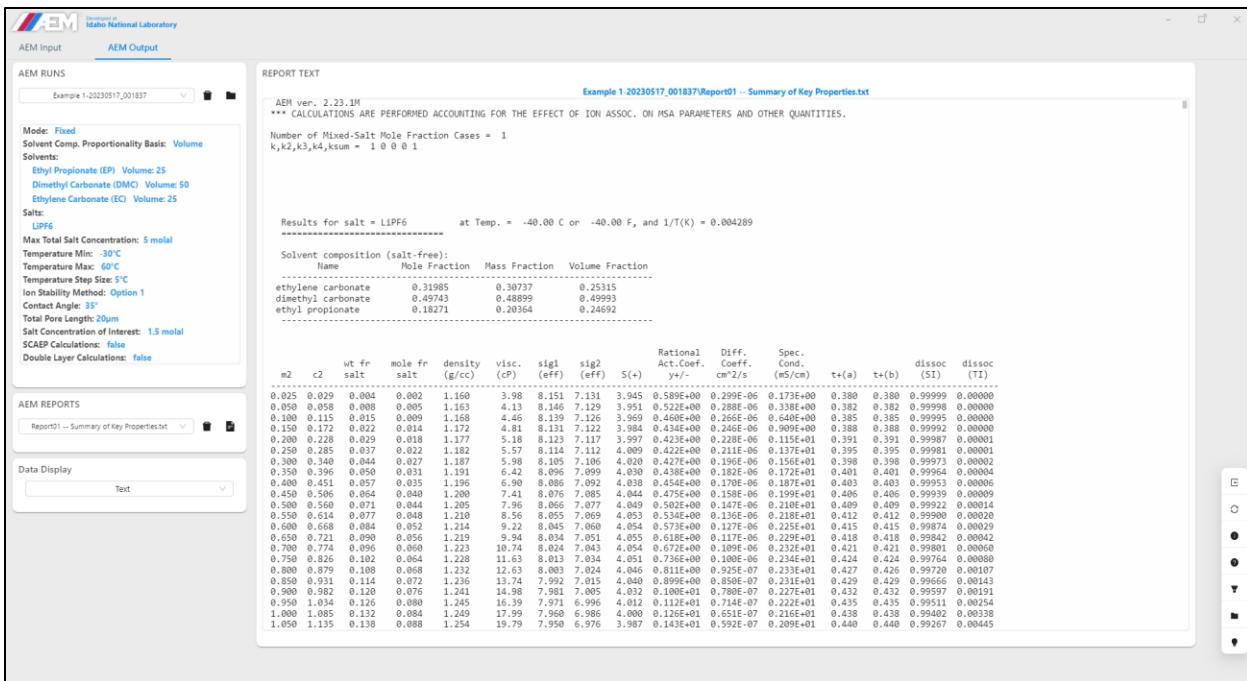
### 4.1.3 Example 1: Data Output & Discussion

Simulation outputs are plotted in Figure 75 - Figure 79 for the transport suite of properties (salt diffusivity, conductivity, viscosity, cation transference number). General goals for battery electrolytes are to achieve high diffusivity and conductivity, low viscosity and high cation transference. Since most property metrics exhibit a strong reliance on salt concentration, an effort should be made to identify the range of salt concentration that maximizes the foremost properties of interest. Note that this range should also consider the possible concentration polarization (CP) that can occur over more prolonged cycling elements, since CP will cause a salt depletion at one electrode, while causing an enrichment at the opposite electrode. Given these factors in concert, a feasible overall operational salt concentration range could be defined as 0.5 to 2.0 molal. Note that the effective temperature range for this example is -40 to 70 °C, since AEM adds temperature steps to enable calculation of activation energies over the user-specified range. Also note that for the cation transference values (Report01), the following is given:

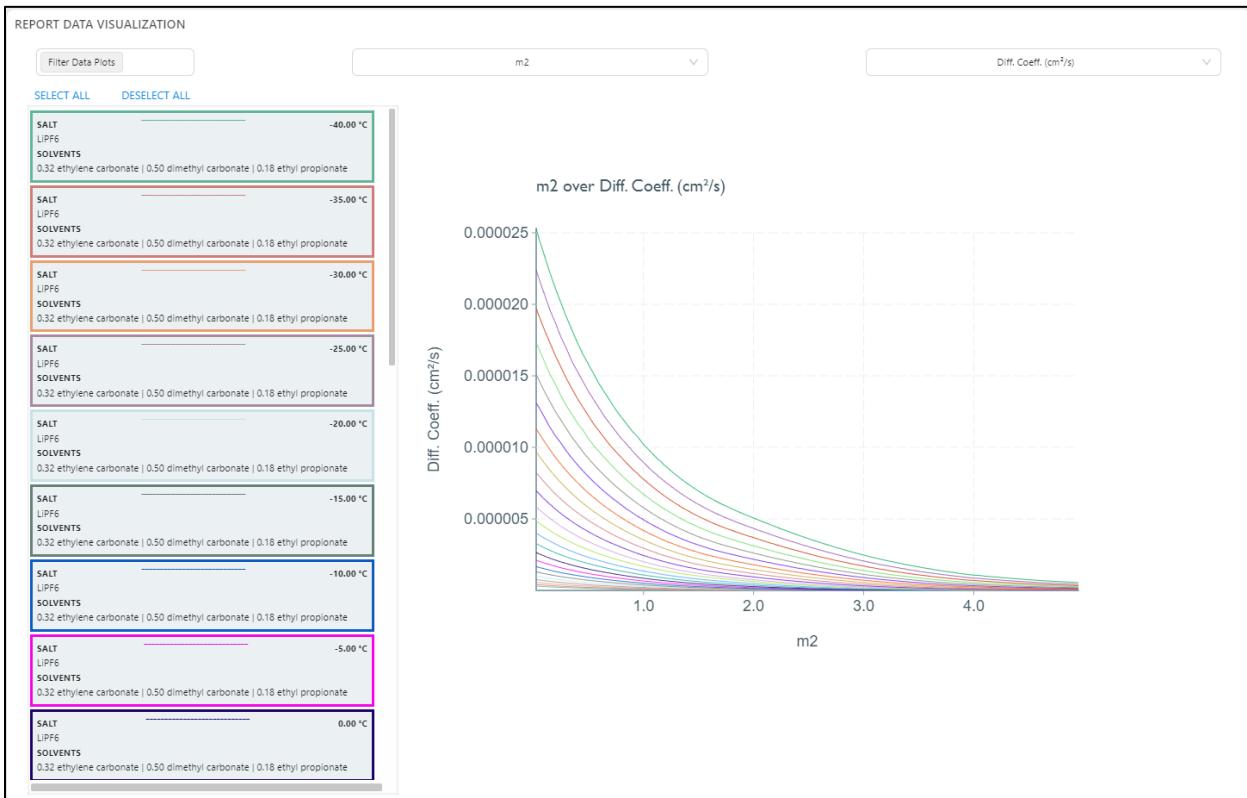
- (a) t+ evaluated with single-ion cations vs all charged species,
- (b) t+ evaluated with all cation-bearing charged species vs all charged species.

The trends seen over these two approaches are very similar, where their behavior over salt concentration reflect the relative change in the local solvating structure around the lithium cations in relation to that of the anions.

## Advanced Electrolyte Model (AEM)

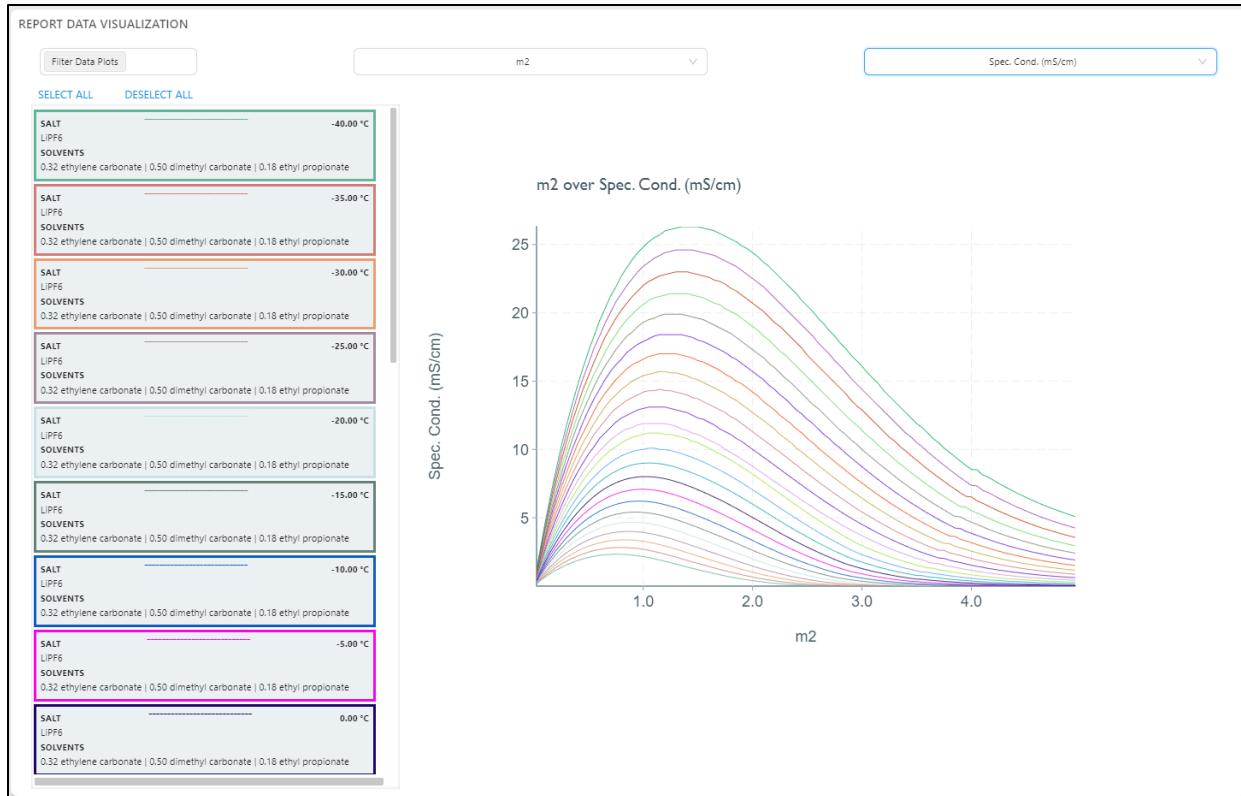


**Figure 74. Example 1 – AEM Output tab – REPORT TEXT section to view Report01–Report20.**

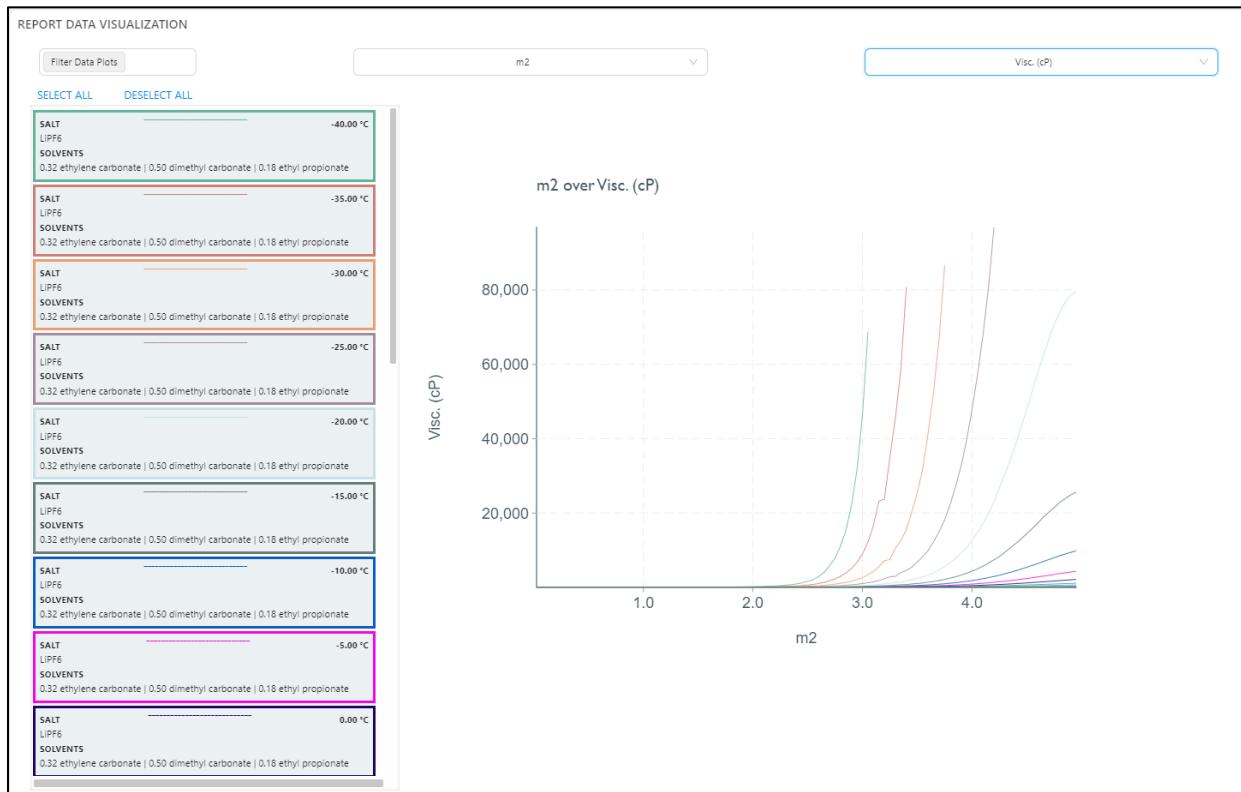


**Figure 75. Example 1 – Diffusivity/Diffusion Coefficient (cm<sup>2</sup>/s) v/s Molal Salt Conc. (m<sup>2</sup>).**

## Advanced Electrolyte Model (AEM)

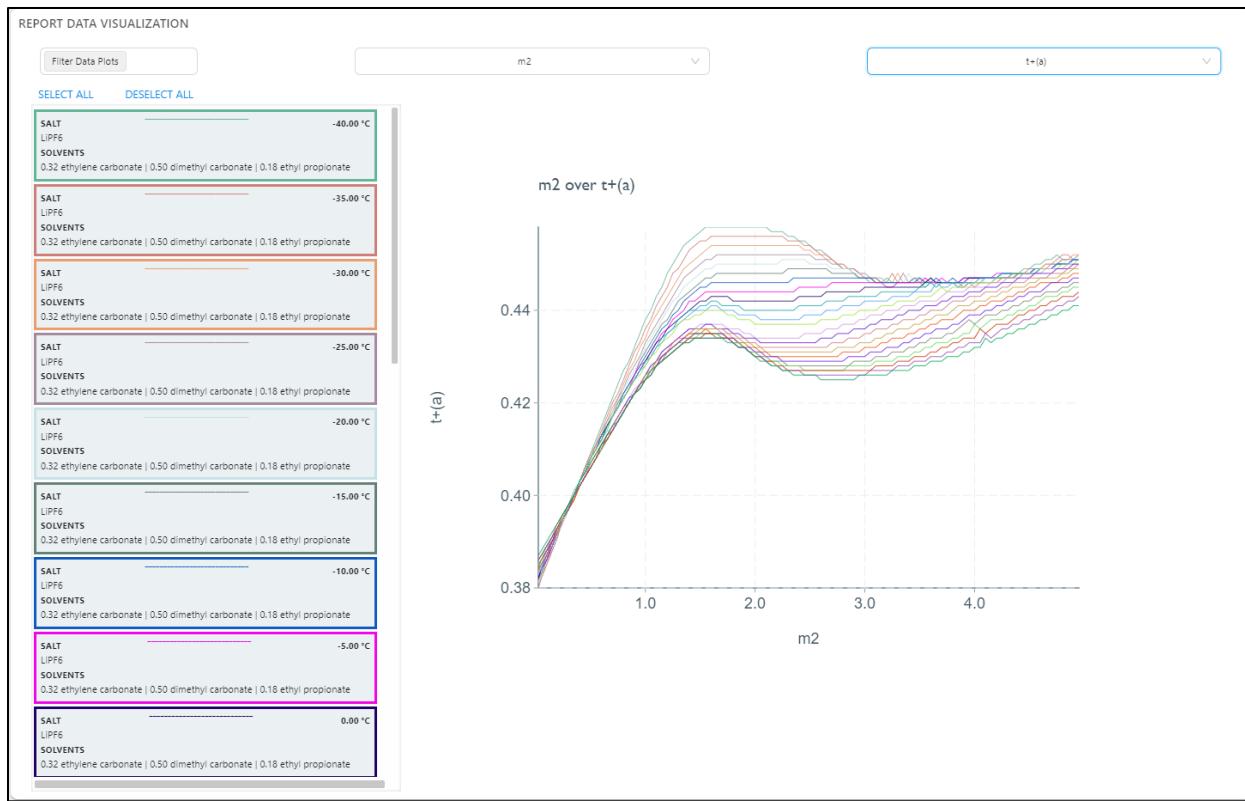


**Figure 76. Example 1 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).**

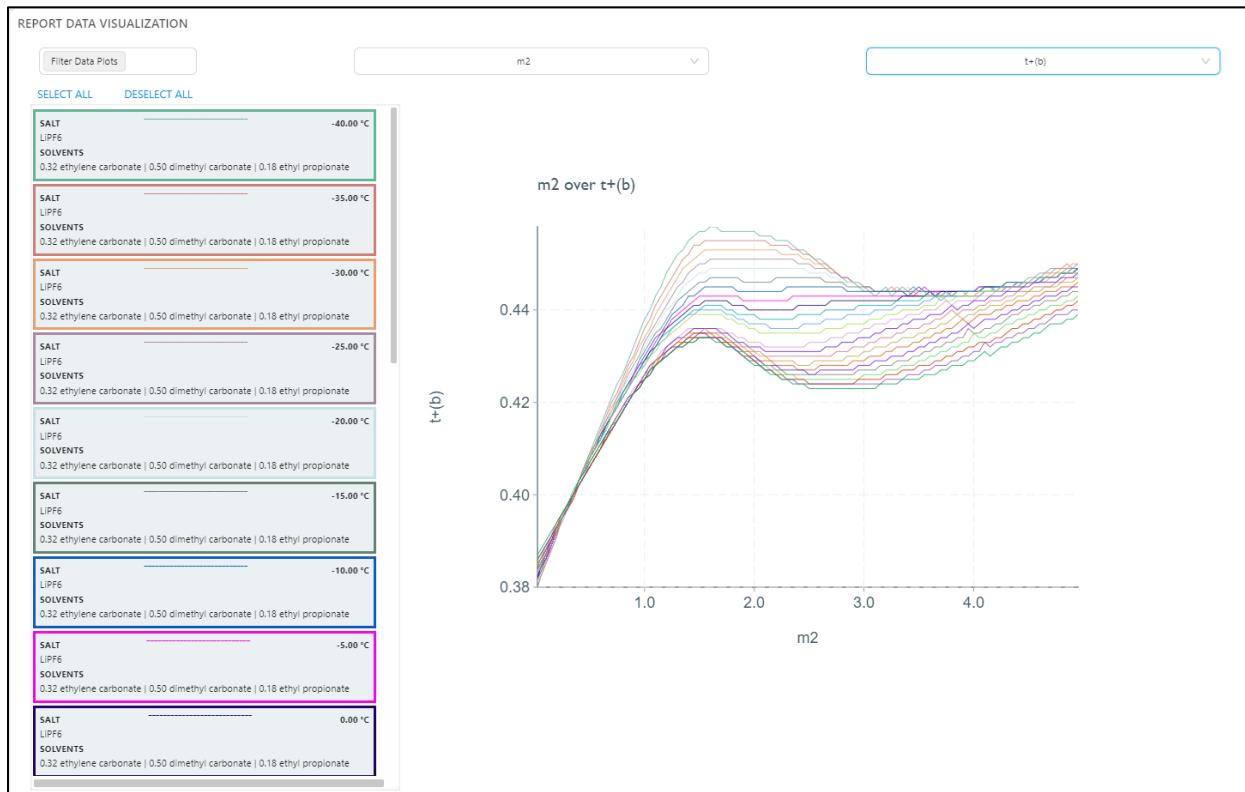


**Figure 77. Example 1 – Viscosity (cP) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)



**Figure 78. Example 1 – Cation Transference No. ( $t+(a)$ ) v/s Molal Salt Conc. ( $m2$ ).**



**Figure 79. Example 1 – Cation Transference No. ( $t+(b)$ ) v/s Molal Salt Conc. ( $m2$ ).**

## 4.2 Example 2: Fixed Mass Proportions for 8-Solvent, 2-Salt System

This example considers a complex eight-solvent system with EC, PC, EMC, MP, DEGDME, BN, TMP, VEC at fixed proportions (10, 10, 15, 20, 25, 12, 5, 3 mass %) with a dual salt LiPF<sub>6</sub> and LiFSI that covers the full dual salt matrix of eleven proportions. The total salt concentration is allowed to go to 5 molal. Other factors behind the simulation include:

- T = 0°C to 50°C with 10°C steps,
- Used default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal,
- No SCAEP; No DL.

The parameters for electrolyte ingress are relevant estimations for battery electrode materials in general and can be updated to reflect more finely tuned attributes of the porous media.

This complex electrolyte represents a lower-viscosity, higher-conductivity system that would facilitate higher current densities in lithium-ion type cells, while adding stability to passivation films (SEI). This electrolyte system has benefits toward conditions like moderately-fast charging and higher-power applications, where the formulation can be fine-tuned through the salt matrix.

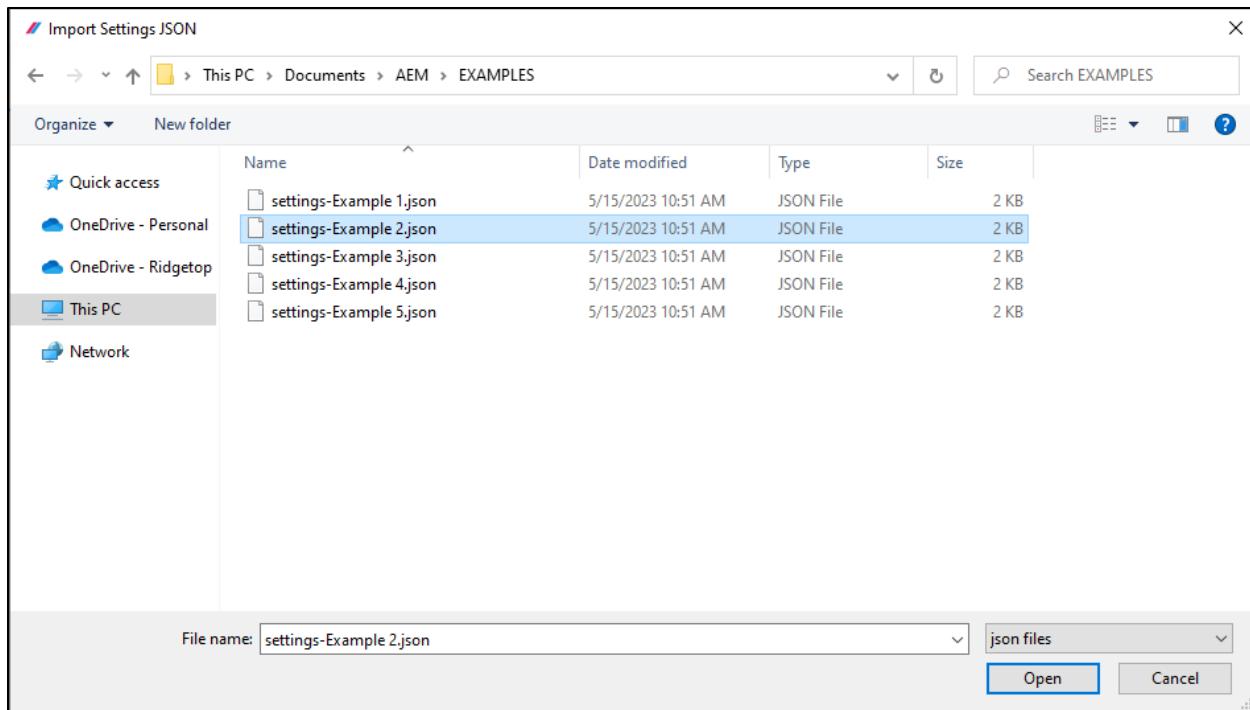
### 4.2.1 Example 2: Importing Example 2 Parameters

We start off Example 2 by first using the **Import** Button from Section 3.5 to prepopulate each of the AEM input conditions for Example 2. This can be achieved by following the list of instructions below and referencing Figure 80 and Figure 81.

- a) Click on the **Import** (Import icon) Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- b) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- c) Select the **settings-Example 2.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 2.json" file was not imported successfully.

## Advanced Electrolyte Model (AEM)



**Figure 80. Importing Example 2 Input Condition using the settings-Example 2.json file.**

### 4.2.2 Example 2: Overview of Simulation Input Conditions

Based on the conditions mentioned at the beginning of this example, select the following

- Select the solvents EC, PC, EMC, MP, DEGDME, BN, TMP, VEC at fixed proportions (10, 10, 15, 20, 25, 12, 5, 3 mass %),
- Select dual salt system LiPF<sub>6</sub> and LiFSI with a total maximum concentration of 5 molal. Choose full dual salt matrix of eleven proportions.
- T = 0°C to 50°C with 10°C steps,
- Use default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal,
- No SCAEP; No DL.

## Advanced Electrolyte Model (AEM)

**SINGLE FIXED COMPOSITION OF SOLVENTS**

**LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION**

**SELECT SOLVENTS**

Volume Mass ⓘ  
Composition Proportionality Basis

Click Solvent from Category to Add:

- WATER
- CARBONATES ⓘ
- DICARBONATES ⓘ
- GLYMES ⓘ
- ESTERS ⓘ
- FROM OTHER CLASSES ⓘ
- S OR P CONTAINING SOLVENTS ⓘ
- NITRILES AND DINITRILES ⓘ
- PHOSPHAZENE ADDITIVES ⓘ

CARBONATES / Ethylene Carbonate (EC)	10	ⓘ
CARBONATES / Propylene Carbonate (PC)	10	ⓘ
CARBONATES / Ethylmethyl Carbonate (EMC)	15	ⓘ
ESTERS / Methyl Propionate (MP)	20	ⓘ
GLYMES / DEGDME (diglyme)	25	ⓘ
NITRILES & DINITRILES / Butyronitrile (BN)	12	ⓘ
S OR P CONTAINING / Trimethyl Phosphate (TMP)	5	ⓘ
CARBONATES / Vinyl Ethylene Carbonate (VEC)	3	ⓘ

**SELECT SALTS**

Single Range ⓘ  
Composition Proportion Mode

Click Salt from Category to Add:

- FOR BATTERY ELECTROLYTES ⓘ
- FOR AQUEOUS SYSTEMS ⓘ
- FOR BATTERY ELECTROLYTES / LiPF6 ⓘ
- FOR BATTERY ELECTROLYTES / LiFSI ⓘ

5 ⓘ  
Max Total Salt Concentration [molal]

**TEMPERATURE SETTINGS**

0 ⓘ Temperature Min [°C] 50 ⓘ Temperature Max [°C] 5 °C 10 °C Temperature Step Size

**METHOD FOR HANDLING TRIPLE ION STABILITY**

$[ABA^+] = [BAB^-]$  (default)  
 $[ABA^+] > [BAB^-]$  due to  $BAB^- \rightarrow B^- + AB$  or  
 $[ABA^+] < [BAB^-]$  due to  $ABA^+ \rightarrow A^+ + AB$   
 (inequalities are automatically determined) ⓘ

**ELECTROLYTE INGRESS INTO PORES**

35 ⓘ Contact Angle [°] 20 ⓘ Total Pore Length [μm] 1.5 ⓘ Salt Concentration of Interest

**SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**

Perform SCAEP Calculations ⓘ

**DOUBLE LAYER (DL)**

Perform DL Calculations ⓘ

**AEM RUN IDENTIFIER (optional)**

Example 2 ⓘ  Append Timestamp

AEM Run Identifier

**Run AEM**

**Figure 81. Example 2 – AEM Input tab.**

### 4.2.3 Example 2: Data Output & Discussion

Simulation outputs are plotted in Figure 83 - Figure 87 for the transport suite of properties (salt diffusivity, conductivity, viscosity, cation transference number). Results are plotted over seven (7) temperatures (0, 10, 20, 30, 40, 50, 60 °C), where at each set of temperature the matrix of eleven (11) dual-salt proportions are included. General goals for battery electrolytes are to achieve high diffusivity and conductivity, low viscosity and high cation transference. While there are similarities between Examples 1 and 2 in the transport properties, Example 2 has the advantage of the additional matrix of dual-salt proportions. Note that favorable salt proportions can change over total salt concentration and temperature. Since most property metrics exhibit a strong reliance on salt concentration, an effort should be made to identify the range of salt concentration that maximizes the foremost properties of interest. Note that this range should also consider the possible concentration polarization (CP) that can occur over more prolonged cycling elements, since CP will cause a salt depletion at one electrode, while causing an enrichment at the opposite electrode. Given these factors in concert, a feasible overall operational salt concentration range could be defined as 0.5 to 2.1 molal. Note that the effective output temperature range for this

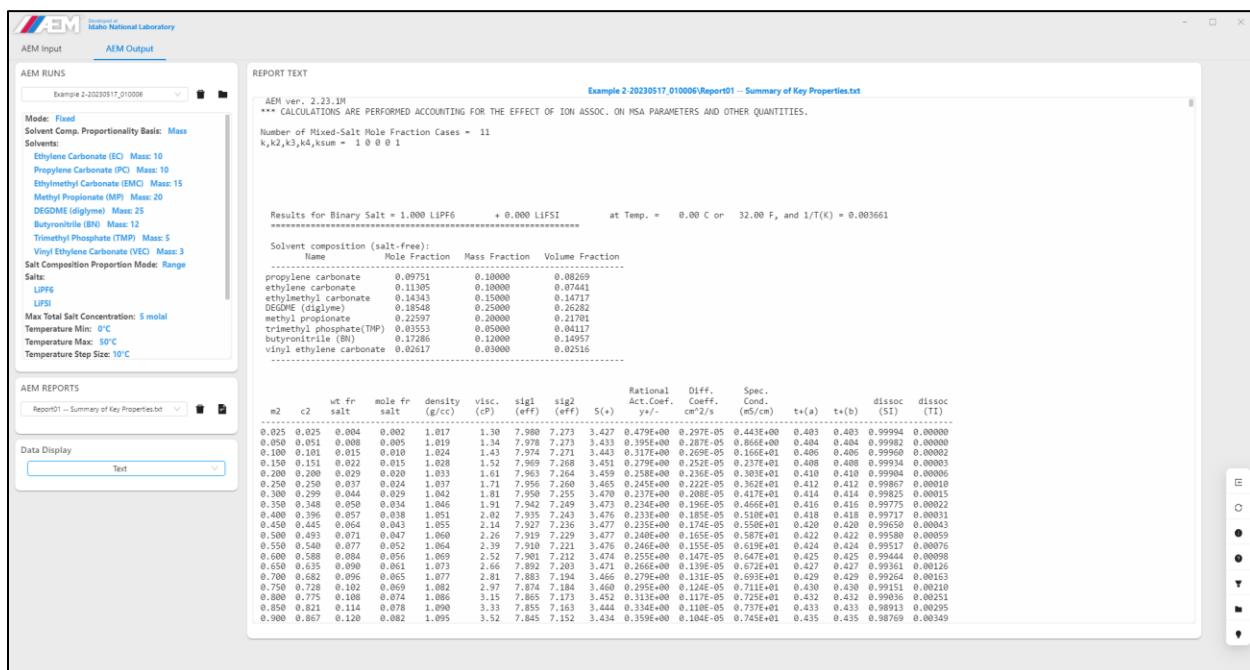
## Advanced Electrolyte Model (AEM)

example is 0 to 60 °C. Also note that for the cation transference values (Report01), the following is given:

(a) t+ evaluated with single-ion cations vs all charged species,

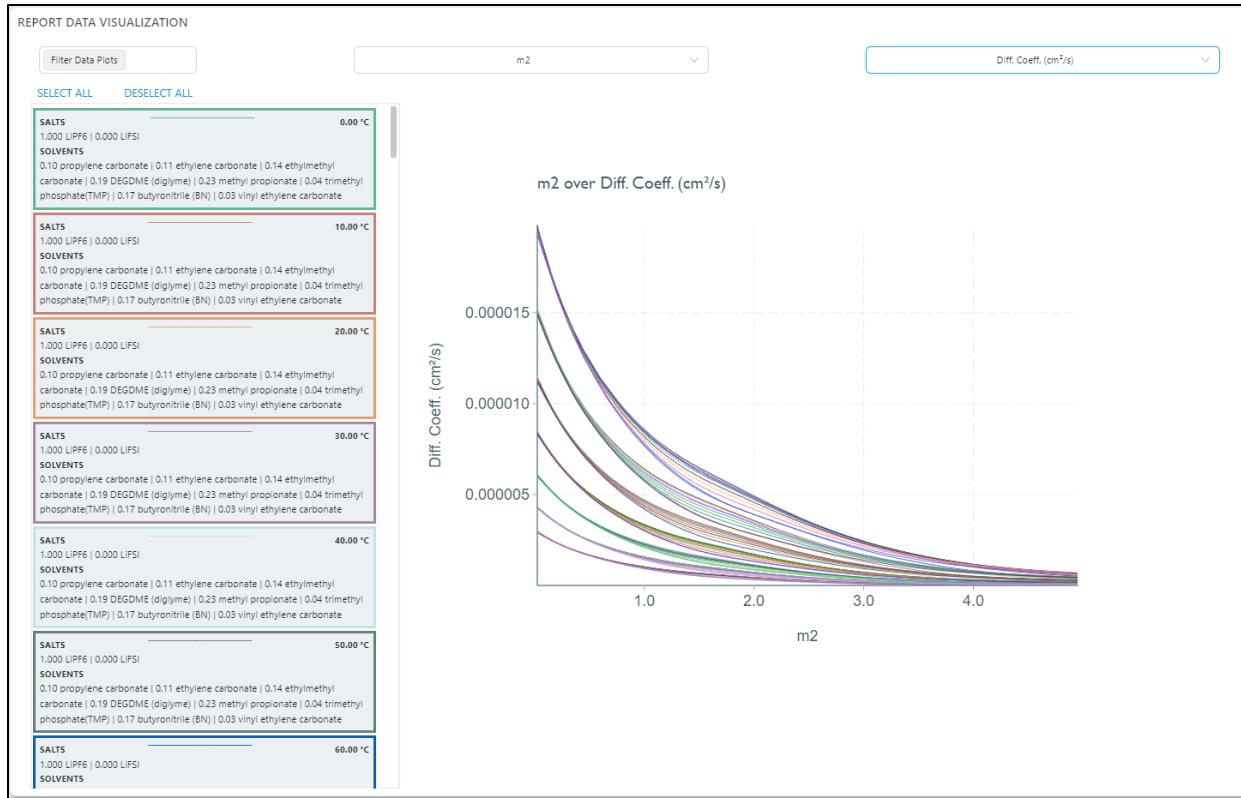
(b) t+ evaluated with all cation-bearing charged species vs all charged species.

The trends seen over these two approaches are very similar, where their behavior over salt concentration reflect the relative change in the local solvating structure around the lithium cations in relation to that of the anions. In Example 2, more variability is seen in t+ over salt concentration compared to Example 1 owing to (1) the more diverse field of solvents that can act as solvators, and (2) the impact of the dual-salt formulations and how the presence of two types of anions affects cation solvation and the corresponding solvated diameter over salt concentration.

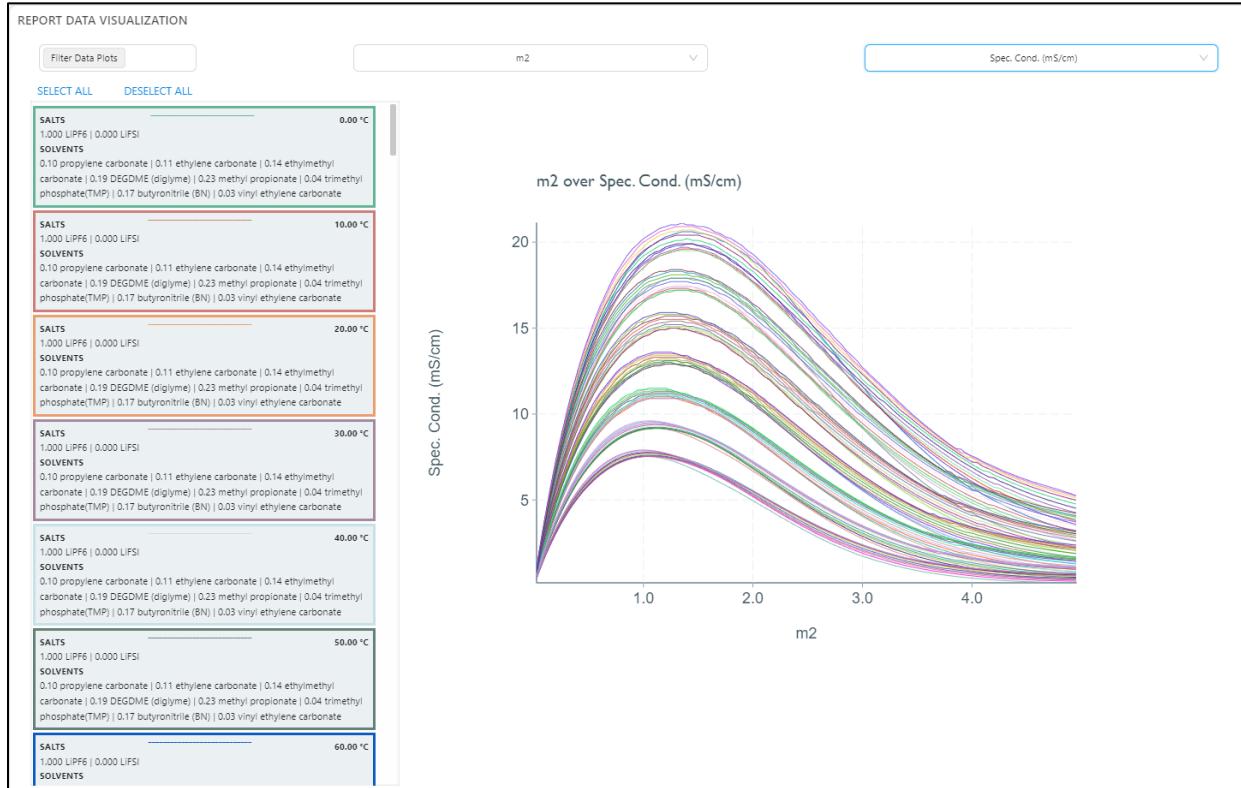


**Figure 82. Example 2 – AEM Output tab – REPORT TEXT section to view Report01-Report20.**

## Advanced Electrolyte Model (AEM)

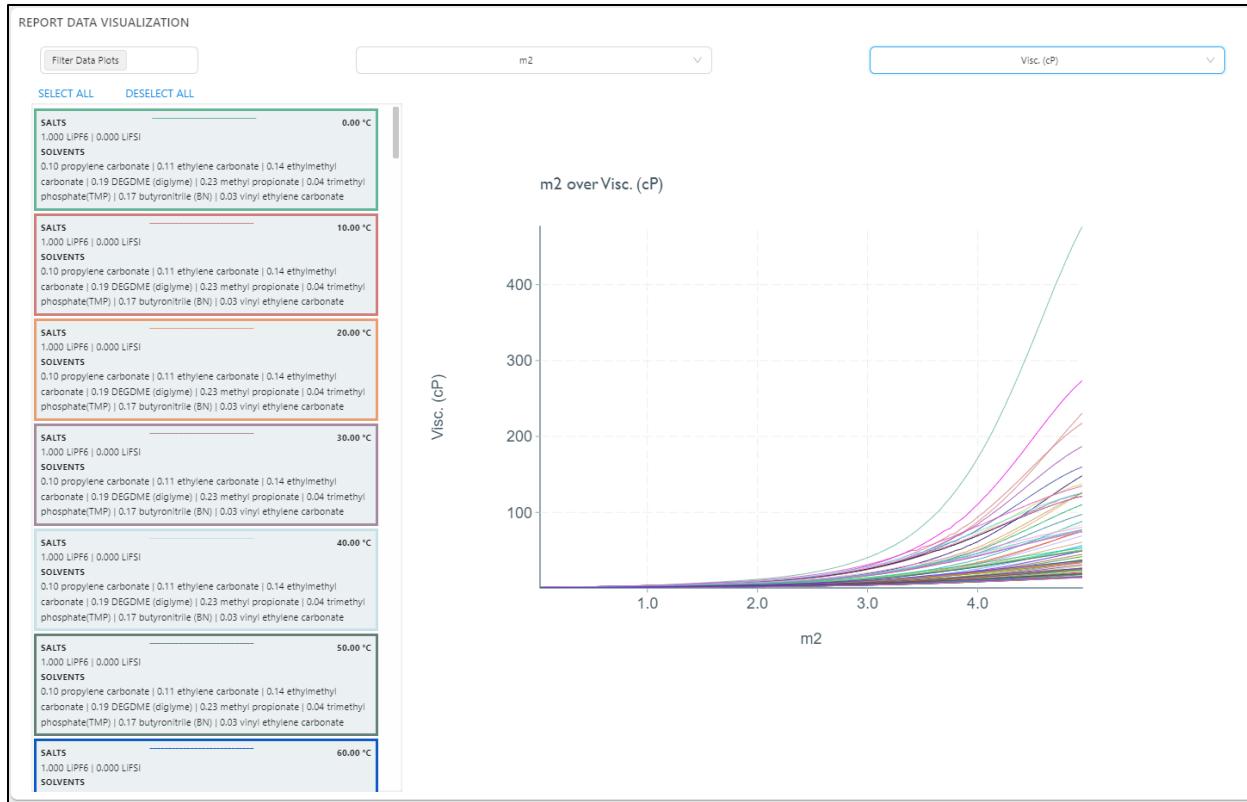


**Figure 83. Example 2 – Diffusivity/Diffusion Coefficient (cm<sup>2</sup>/s) v/s Molal Salt Conc. (m2).**

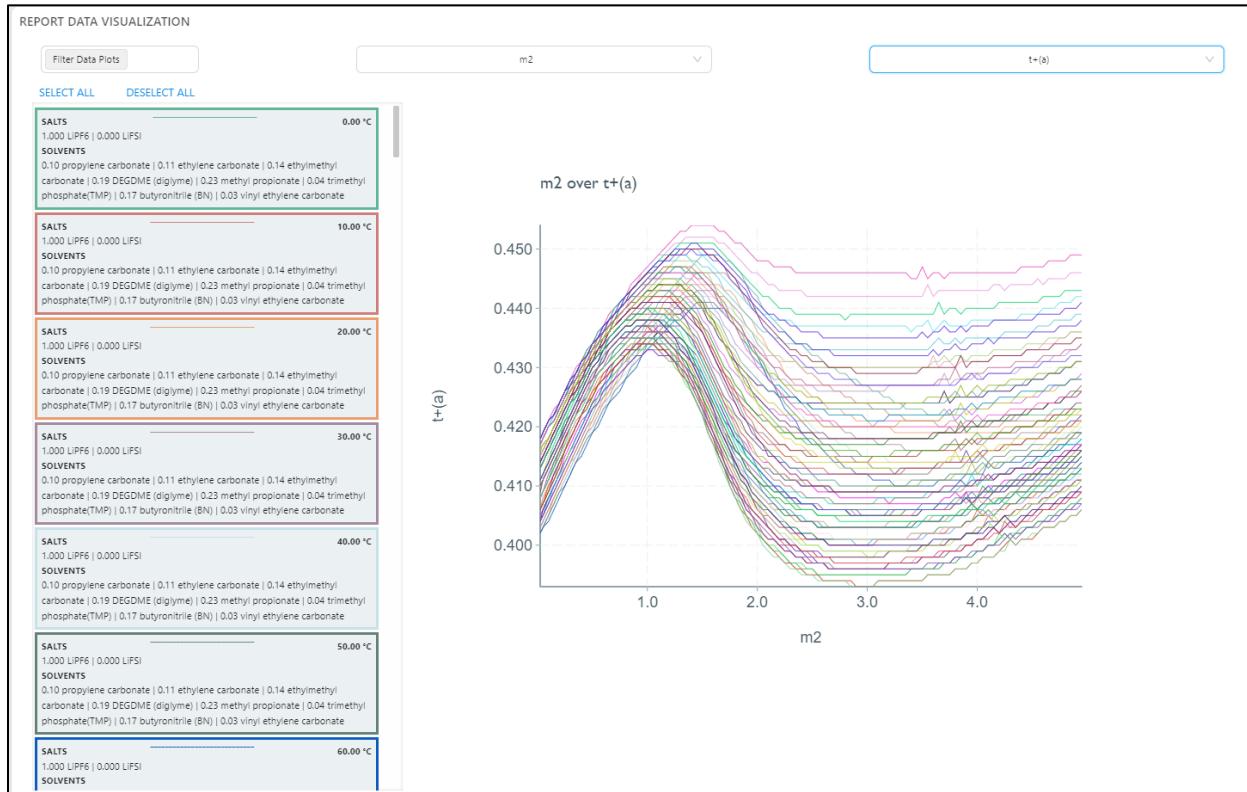


**Figure 84. Example 2 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)

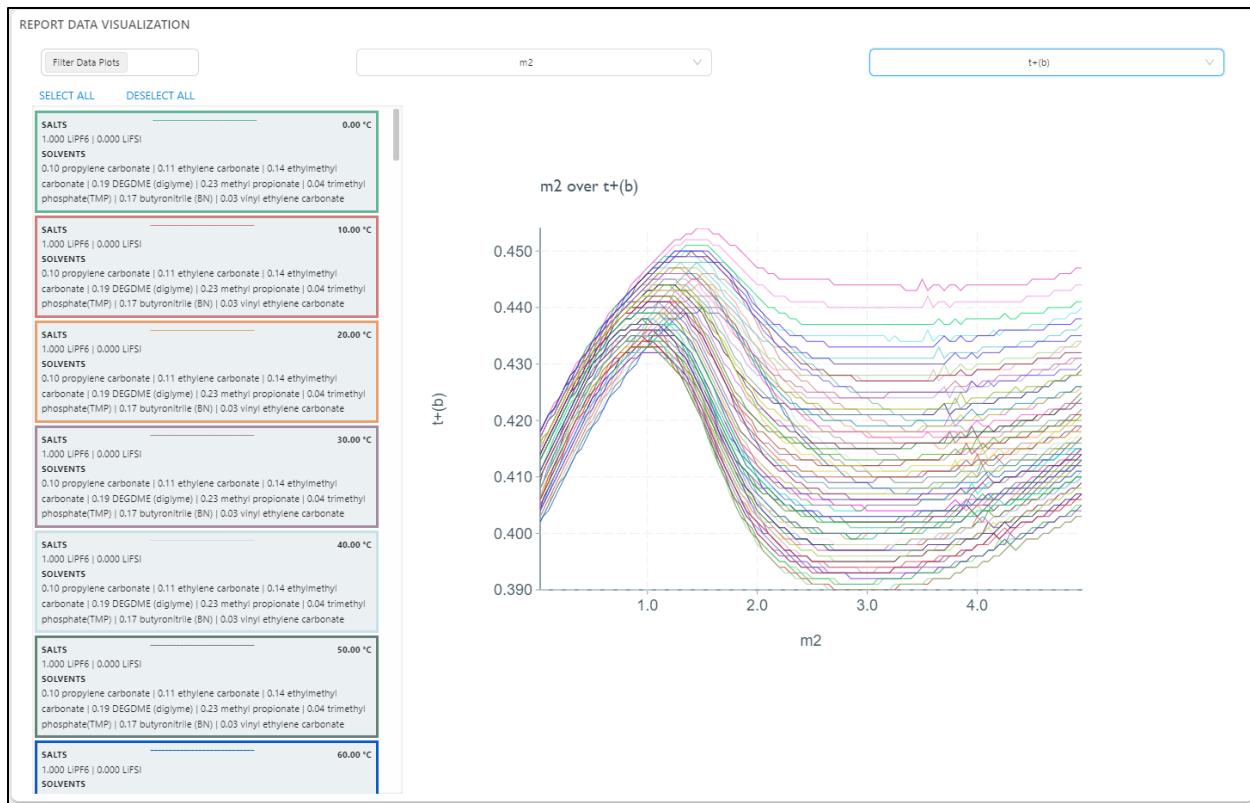


**Figure 85. Example 2 – Viscosity (cP) v/s Molal Salt Conc. (m2).**



**Figure 86. Example 2 – Cation Transference No. (t+(a)) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)



**Figure 87. Example 2 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. ( $m_2$ ).**

## 4.3 Example 3: 3-Solvent with Fixed Volume Proportions and

This example is similar to Example 1, yet with a fixed dual salt and higher maximum salt concentration. Considered is the three-solvent system EC, DMC, EP at a fixed volume fraction composition (25, 50, 25 vol %) with LiPF<sub>6</sub> and LiBF<sub>4</sub>. The total salt concentration is allowed to go to 7 molal. Other factors behind the simulation include:

- T = -20°C to 50°C with 5°C steps,
- Used default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal,
- Yes SCAEP; No DL.

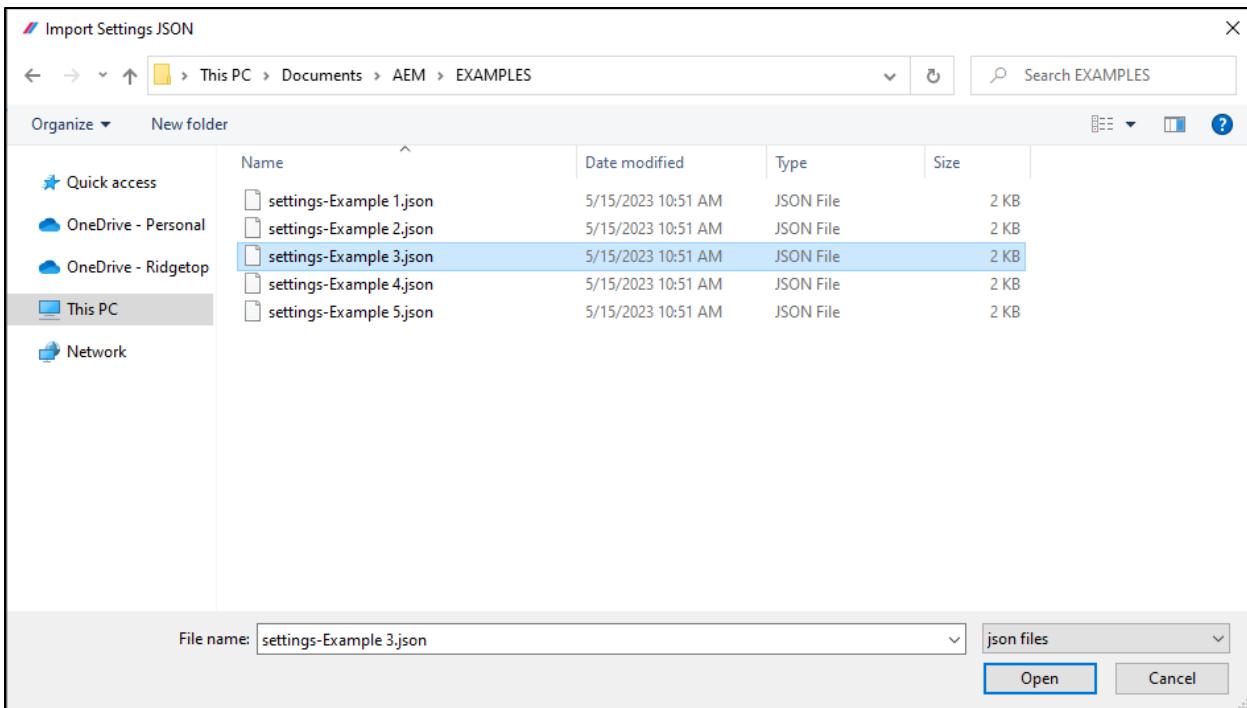
This relatively simple electrolyte represents a lower-viscosity, higher-conductivity system that would facilitate higher current densities in lithium-ion type cells, with possible benefits past Example 1 due to the mixed salts. This electrolyte system has benefits toward conditions like moderately-fast charging and higher-power applications. A key difference in this example is that at the higher salt concentrations (generally past 5 molal) the AEM software detects more cases of "possible onset of solid phase formation", which impacts calculations thereafter that may discover interesting trends in terms like viscosity and conductivity.

### 4.3.1 Example 3: Importing Example 3 Parameters

We start off Example 3 by first using the **Import** Button from Section 3.5 to prepopulate each of the AEM input conditions for Example 3. This can be achieved by following the below list of instructions and referencing Figure 88 and Figure 89.

- a) Click on the **Import** (Import icon) Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- b) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- c) Select the **settings-Example 3.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 3.json" file was not imported successfully.



**Figure 88. Importing Example 3 Input Condition using the settings-Example 3.json file.**

### 4.3.2 Example 3: Overview of Simulation Input Conditions

Based on the conditions mentioned at the beginning of this example, select the following

- Select the three-solvent system EC, DMC, EP at a fixed volume fraction composition (25, 50, 25 vol %)
- Select the dual salt LiPF<sub>6</sub> and LiBF<sub>4</sub> (70:30 molar proportions), where the maximum salt concentration is 7 molal,
- Choose T = -20°C to 50°C with 5°C steps,
- Used default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal,
- Yes SCAEP; No DL. This will generate Report10, which contains information on how the magnitude of the electrode surface charge density will attenuate the relative permittivity of the neighboring electrolyte. The following SCAEP inputs are used:
  - a. Mode 1 (discharge)
  - b. Voltage = 4.2V
  - c. Conc. = 2.0
  - d. SEI thickness = 250.
  - e. SEI relative permittivity = 12.
  - f. SEI porosity = 0.3

## Advanced Electrolyte Model (AEM)

**SINGLE FIXED COMPOSITION OF SOLVENTS**

LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION

**SELECT SOLVENTS**

Volume | Mass ⓘ Composition Proportionality Basis

Click Solvent from Category to Add:

- WATER
- CARBONATES ⓘ
- DICARBONATES ⓘ
- GLYMES ⓘ
- ESTERS ⓘ
- FROM OTHER CLASSES ⓘ
- S OR P CONTAINING SOLVENTS ⓘ
- NITRILES AND DINITRILES ⓘ
- PHOSPHAZENE ADDITIVES ⓘ

CARBONATES / Ethylene Carbonate (EC)	25	ⓘ
CARBONATES / Dimethyl Carbonate (DMC)	50	ⓘ
ESTERS / Ethyl Propionate (EP)	25	ⓘ

**SELECT SALTS**

Single Range ⓘ Composition Proportion Mode

Click Salt from Category to Add:

- FOR BATTERY ELECTROLYTES ⓘ
- FOR AQUEOUS SYSTEMS ⓘ

FOR BATTERY ELECTROLYTES / LiPF6	70	ⓘ
FOR BATTERY ELECTROLYTES / LiBF4	30	ⓘ

7 ⓘ Max Total Salt Concentration [molar]

**TEMPERATURE SETTINGS**

-20 ⓘ 50 ⓘ 5 °C 10 °C Temperature Step Size

Temperature Min [°C] Temperature Max [°C]

**METHOD FOR HANDLING TRIPLE ION STABILITY**

[ABA<sup>+</sup>] = [BAB<sup>-</sup>] (default) [ABA<sup>+</sup>] > [BAB<sup>-</sup>] due to BAB<sup>-</sup> → B<sup>-</sup> + AB or [ABA<sup>+</sup>] < [BAB<sup>-</sup>] due to ABA<sup>+</sup> → A<sup>+</sup> + AB (inequalities are automatically determined) ⓘ

**ELECTROLYTE INGRESS INTO PORES**

35 ⓘ 20 ⓘ 1.5 ⓘ Contact Angle [°] Total Pore Length [μm] Salt Concentration of Interest

**SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**

Perform SCAEP Calculations ⓘ

Discharge	Charge	4.2 ⓘ	2.0 ⓘ
Type of Pulse Condition	Cell Voltage of Interest [V]	Bulk Salt Concentration [m]	

250 ⓘ	12 ⓘ	0.3 ⓘ
Thickness of Cathode SEI [Å]	Rel. Permittivity of Cathode SEI [%]	Ave. Porosity of Cathode SEI [%]

**DOUBLE LAYER (DL)**

Perform DL Calculations ⓘ

**AEM RUN IDENTIFIER (optional)**

Example 3 ⓘ  Append Timestamp

AEM Run Identifier

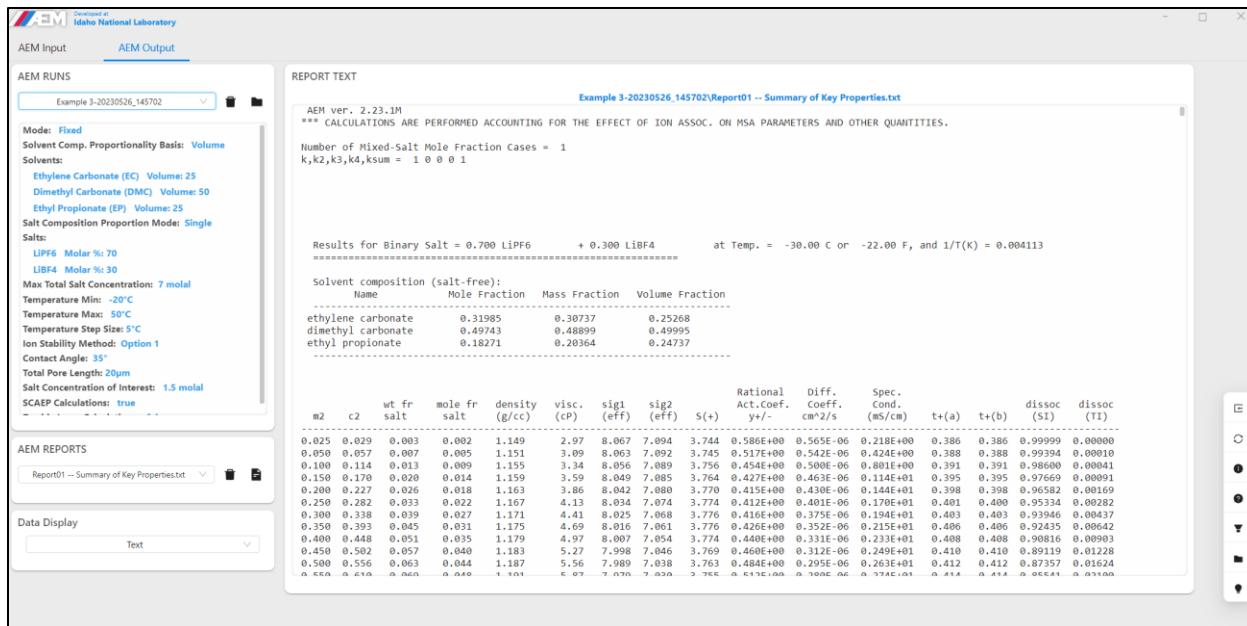
**Run AEM**

**Figure 89. Example 3 – AEM Input tab.**

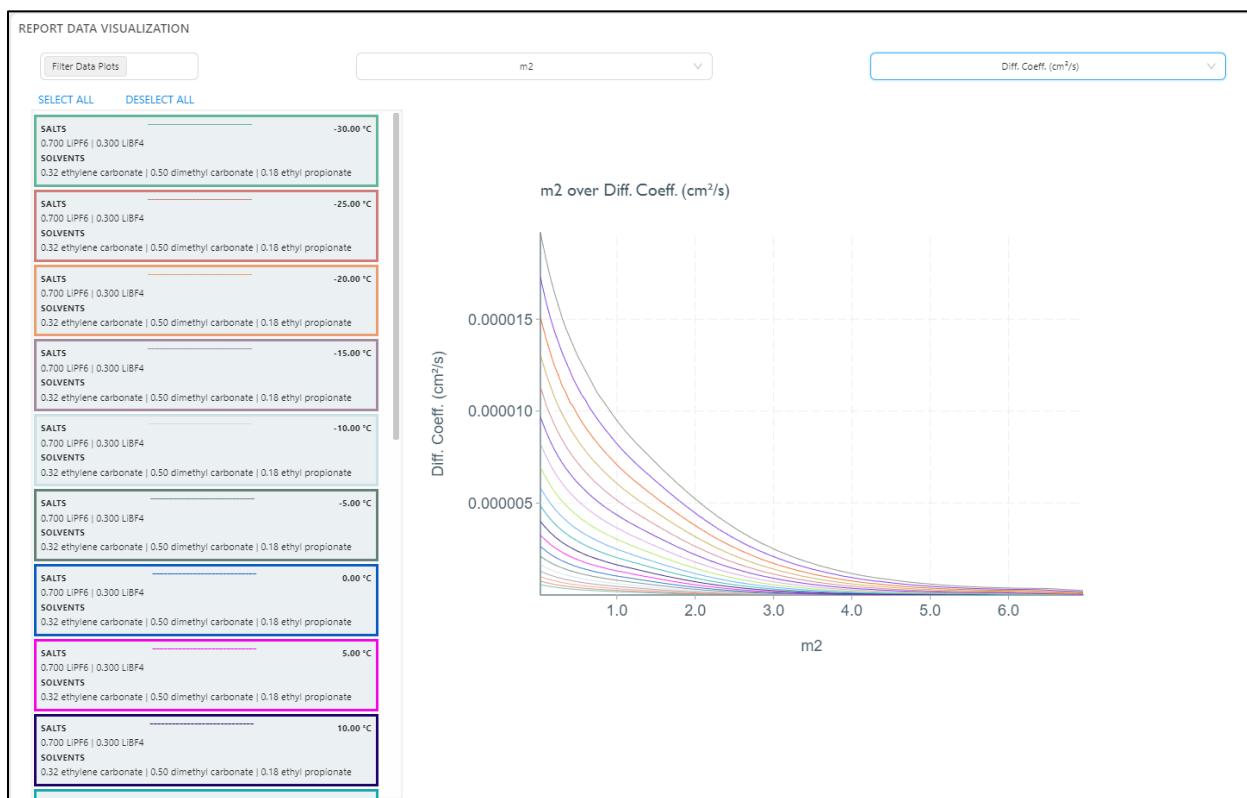
### 4.3.3 Example 3: Data Output & Discussion

Discussion of this example is similar to Example 1, with the following distinction. The presence of LiBF<sub>4</sub> (30% molar in total salt) causes a higher incidence of ion association due to the smaller anion size compared to PF<sub>6</sub><sup>-</sup>, which reduces the amount of free ion charge carriers in solution. As a result, ionic conductivity values are lower than for Example 1, yet the viscosity is generally lower, and the salt diffusivity is higher. Thus, this example showcases the impact of introducing a salt like LiBF<sub>4</sub> that has an anion with a smaller size. Aside from transport properties, potential benefits may arise from mixed salt electrolytes in terms of reduced cation desolvation energies. Figure 90 - Figure 95 cover this example case.

# Advanced Electrolyte Model (AEM)

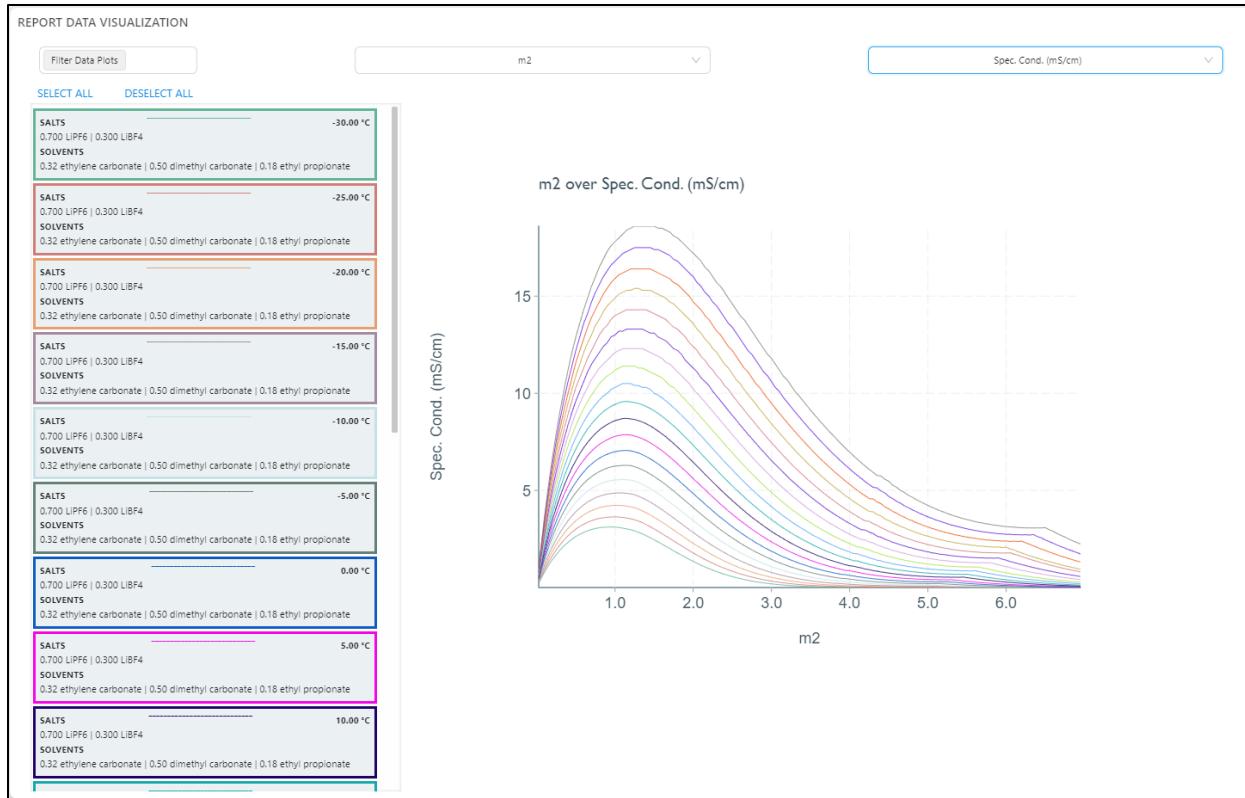


**Figure 90. Example 3 – AEM Output tab – REPORT TEXT section to view Report01–Report20.**

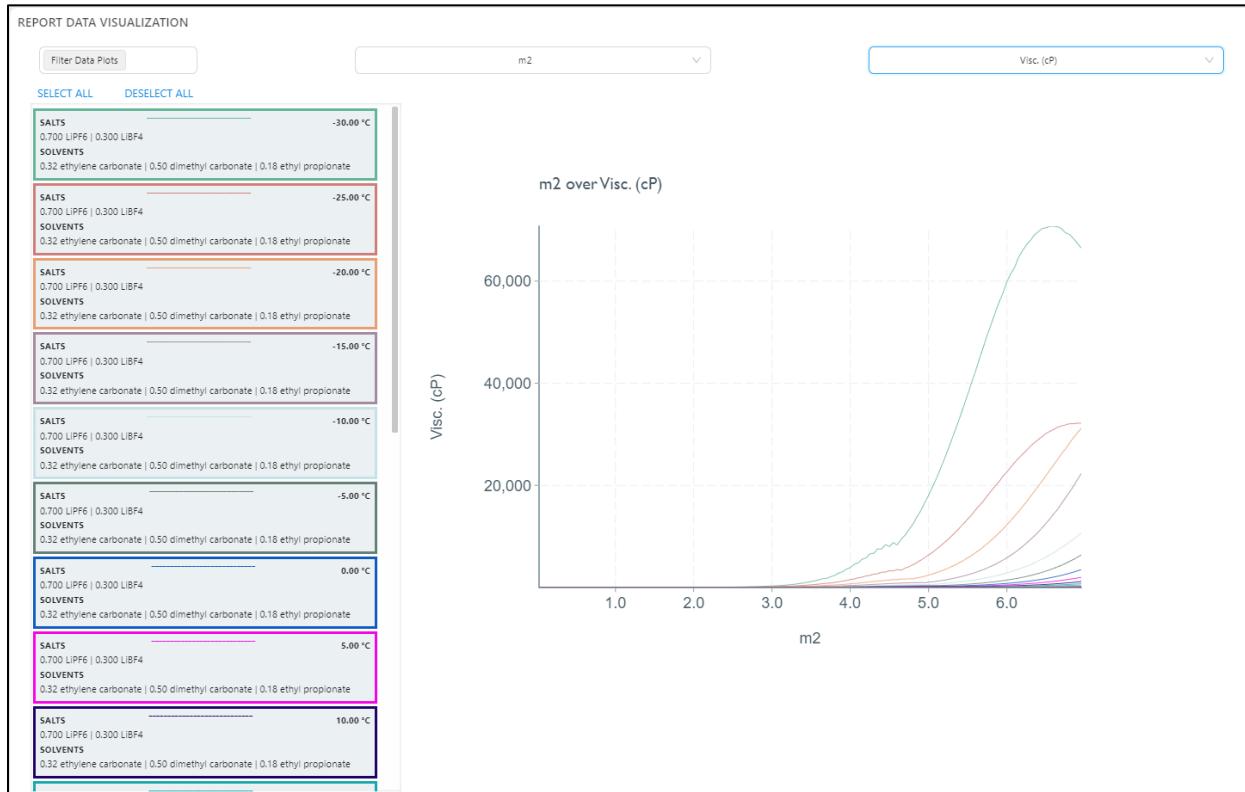


**Figure 91. Example 3 – Diffusivity/Diffusion Coefficient ( $\text{cm}^2/\text{s}$ ) v/s Molal Salt Conc. ( $m_2$ ).**

## Advanced Electrolyte Model (AEM)

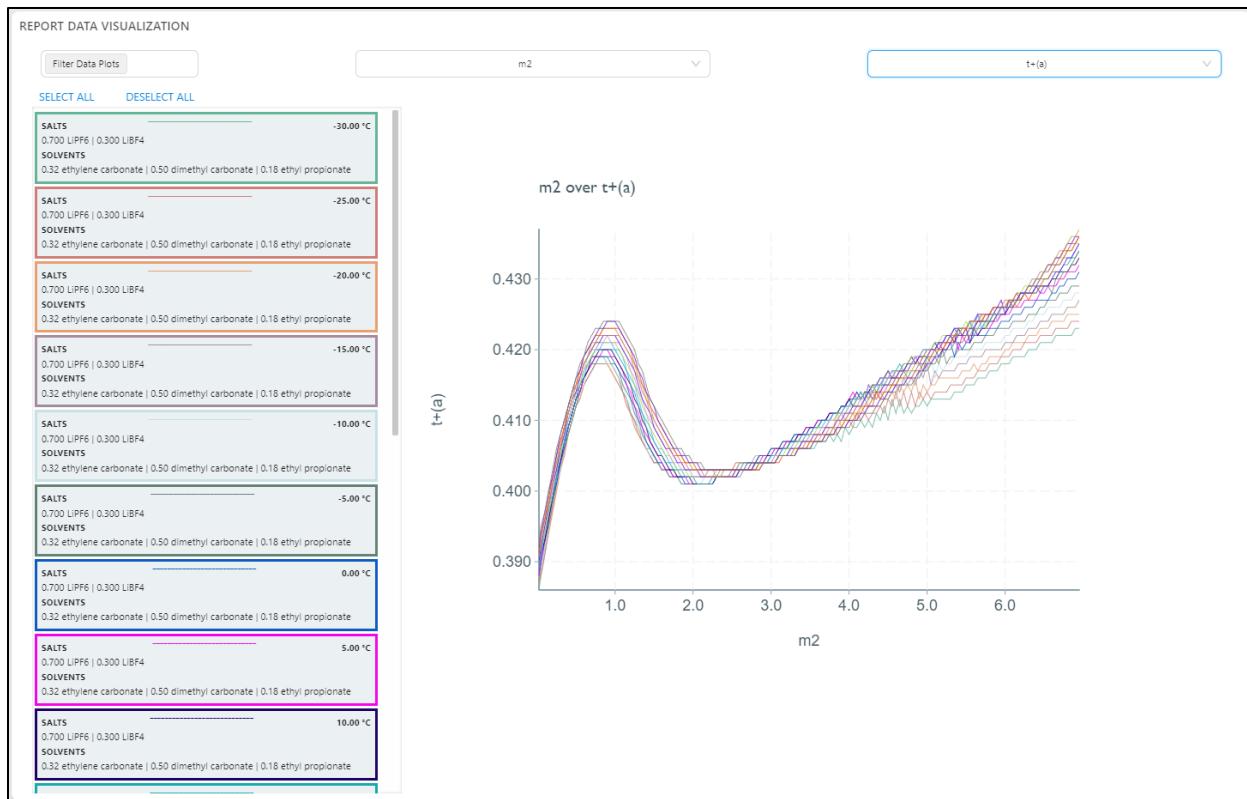


**Figure 92. Example 3 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).**

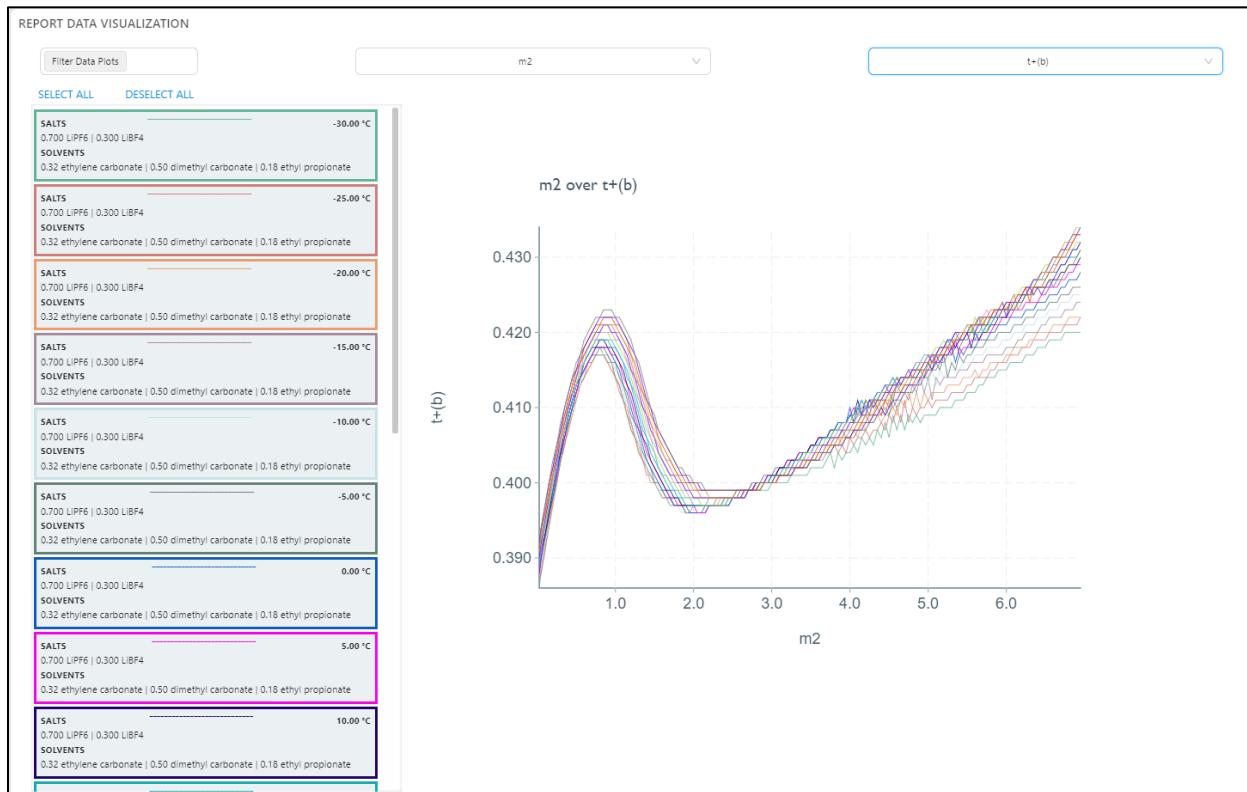


**Figure 93. Example 3 – Viscosity (cP) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)



**Figure 94. Example 3 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. (m2).**



**Figure 95. Example 3 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. (m2).**

## 4.4 Example 4: Water-based 2-Salt System with Fixed Molar Proportion

Aqueous chemistry research can see strong benefits from AEM. This example considers a dual salt system  $\text{LiNO}_3 + \text{Na}_2\text{SO}_4$  of equimolar amounts in water. The effective total salt concentration approaches 12 molal. Other input factors for simulation of this system:

- $T = 0^\circ\text{C}$  to  $70^\circ\text{C}$  with  $10^\circ\text{C}$  steps;
- Use default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle =  $35^\circ$ , Pore length =  $20\mu\text{m}$ , salt conc. of interest = 1.5 molal
- No SCAEP; No DL.

An example of this type demonstrates AEM capabilities at higher salt concentrations than are ordinarily found for non-aqueous battery electrolytes.

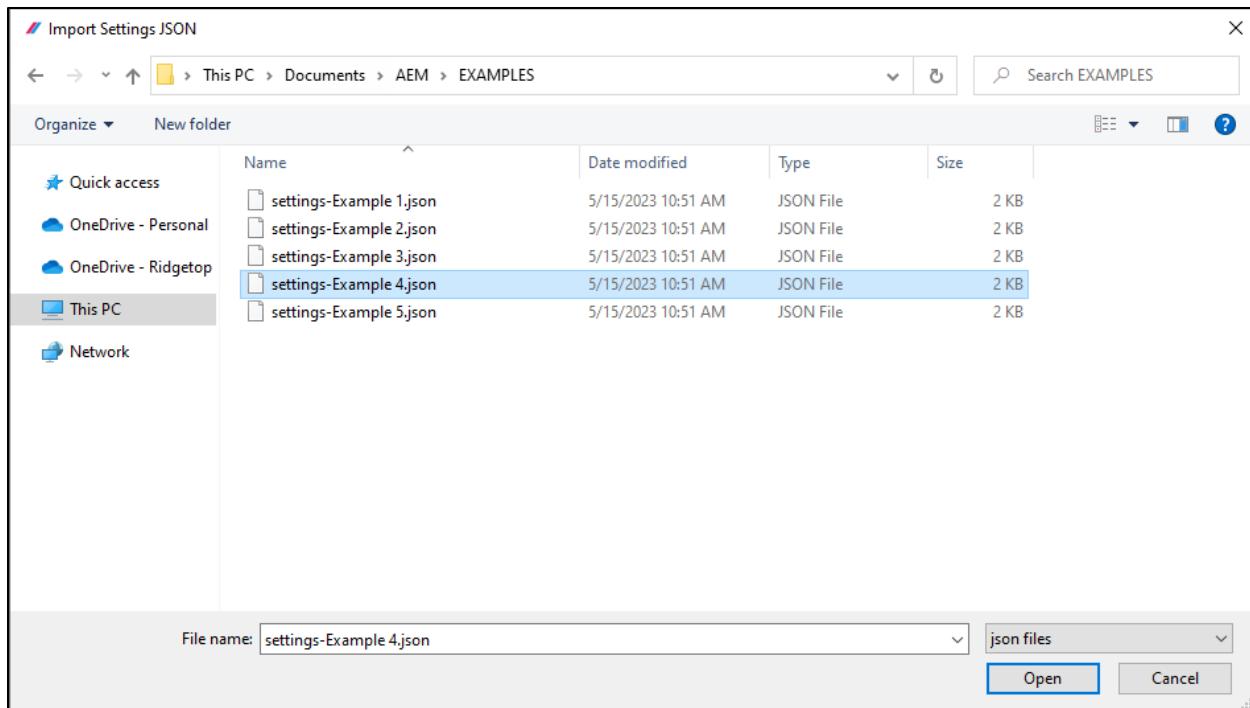
### 4.4.1 Example 4: Importing Example 4 Parameters

We start off Example 4 by first using the **Import** Button from section 3.5 to prepopulate each of the AEM input conditions for Example 4. This can be achieved by following the list of below instructions and referencing Figure 96 and Figure 97.

- a) Click on the **Import** (Import icon) Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- b) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- c) Select the **settings-Example 4.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 4.json" file was not imported successfully.

## Advanced Electrolyte Model (AEM)



**Figure 96. Importing Example 4 Input Condition using the settings-Example 5.json file.**

### 4.4.2 Example 4: Overview of Simulation Input Conditions

- Choose water as the solvent,
- Choose the dual salt system LiNO<sub>3</sub> + Na<sub>2</sub>SO<sub>4</sub> of equimolar amounts (50:50); specify 15 molal total salt (*this is different than the output range of approximately 12 molal, since AEM determines what is feasible given a combination of the 1:1 and 1:2 type salts*),
- Specify T = 0°C to 70°C with 10°C steps
- Use default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal
- Choose No SCAEP; No DL.

## Advanced Electrolyte Model (AEM)

**SINGLE FIXED COMPOSITION OF SOLVENTS**

**LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION**

**TEMPERATURE SETTINGS**

Temperature Min [°C] 0, Temperature Max [°C] 70, Temperature Step Size 5 °C to 10 °C

**METHOD FOR HANDLING TRIPLE ION STABILITY**

[ABA\*] = [BAB\*] (default)    [ABA\*] > [BAB\*] due to BAB- → B+ + AB or [ABA\*] < [BAB\*] due to ABA\* → A+ + AB (inequalities are automatically determined)

**ELECTROLYTE INGRESS INTO PORES**

Contact Angle [°] 35, Total Pore Length [μm] 20, Salt Concentration of Interest 1.5

**SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**

Perform SCAEP Calculations

**DOUBLE LAYER (DL)**

Perform DL Calculations

**AEM RUN IDENTIFIER (optional)**

Example 4,  Append Timestamp

Max Total Salt Concentration [molar] 15

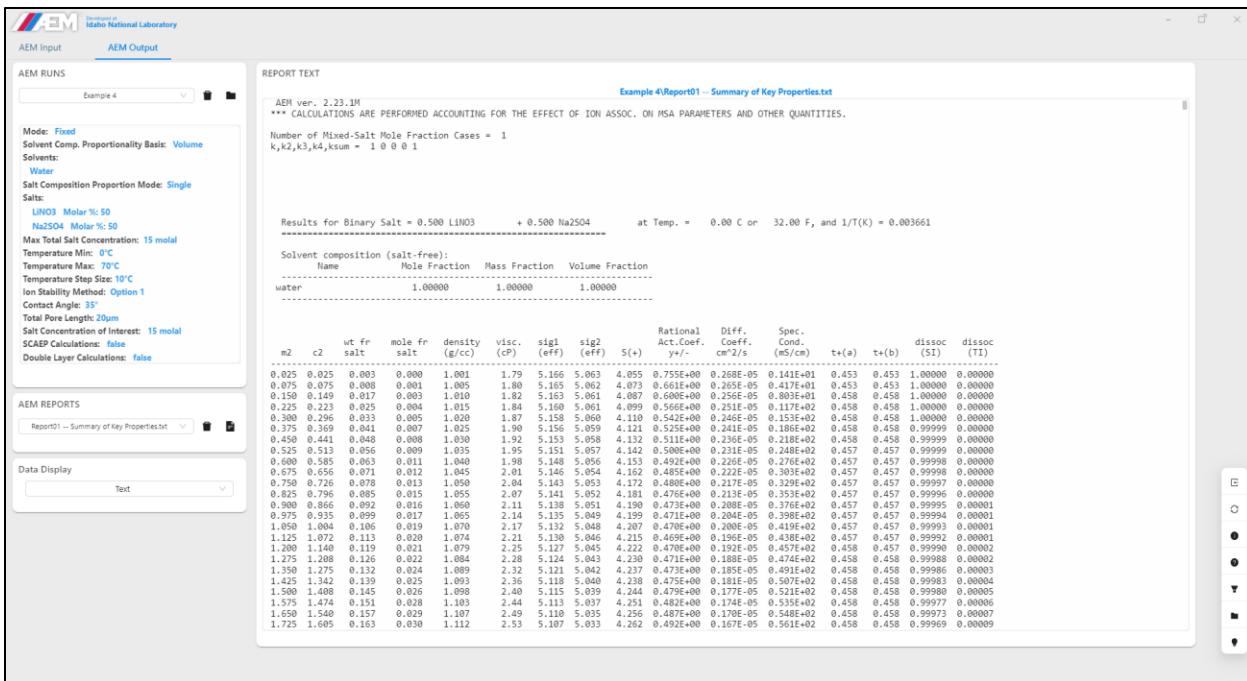
Run AEM

**Figure 97. Example 4 – AEM Input tab.**

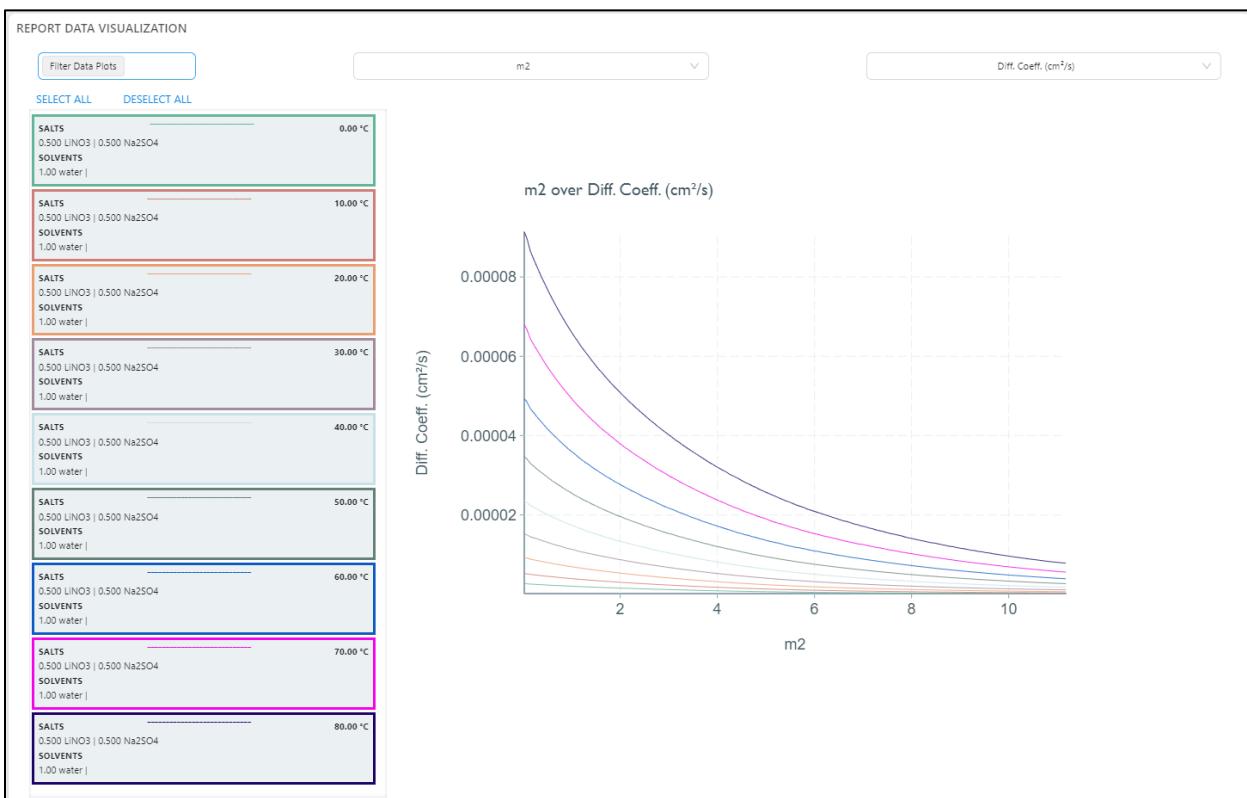
### 4.4.3 Example 4: Data Output & Discussion

Figure 99 - Figure 103 summarize the transport plots for this example. Whether for aqueous battery systems or water treatment applications, the collection of output properties generated within the twenty (20) reports gives genomic data for aqueous systems. This example demonstrates that AEM can operate at elevated salt content while considering different salt stoichiometries (here, 1:1 and 1:2 in the same system).

## Advanced Electrolyte Model (AEM)

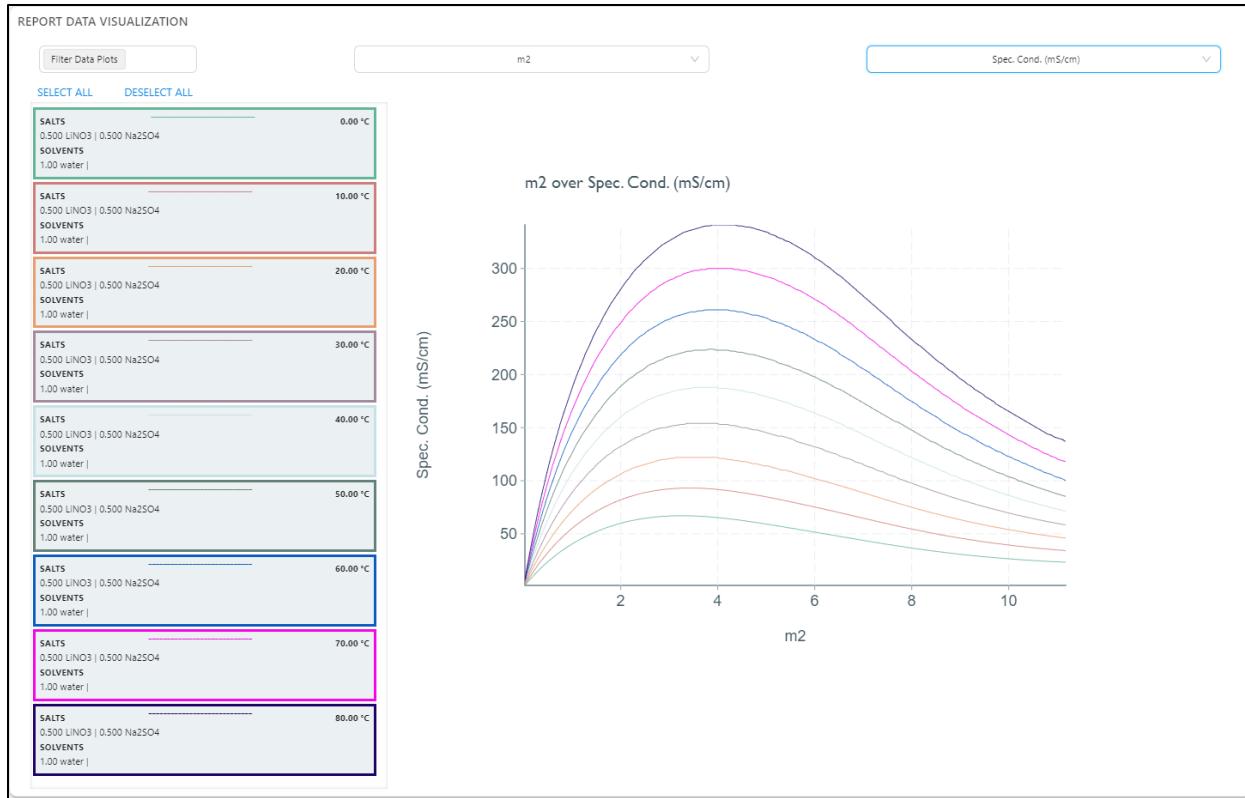


**Figure 98. Example 4 – AEM Output tab – REPORT TEXT section to view Report01–Report20.**

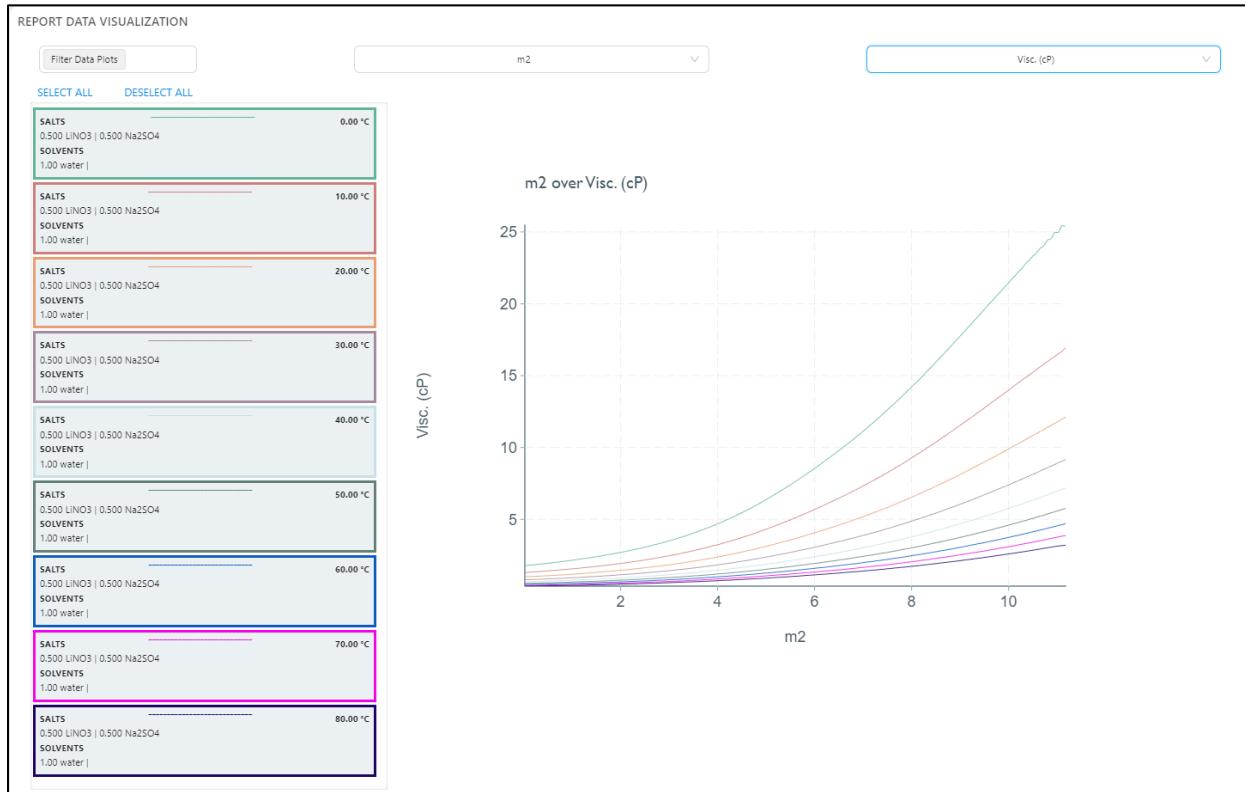


**Figure 99. Example 4 – Diffusivity/Diffusion Coefficient (cm<sup>2</sup>/s) v/s Molal Salt Conc. (m<sub>2</sub>).**

## Advanced Electrolyte Model (AEM)

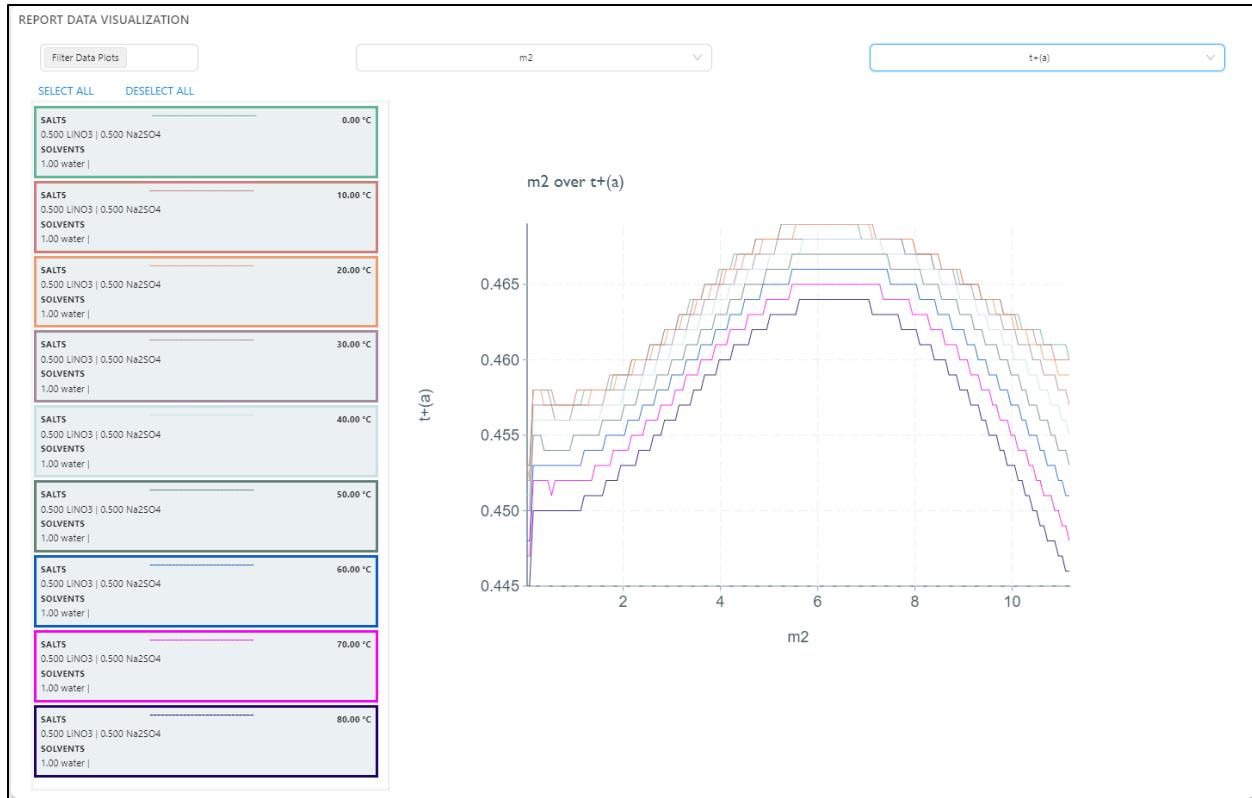


**Figure 100. Example 4 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).**

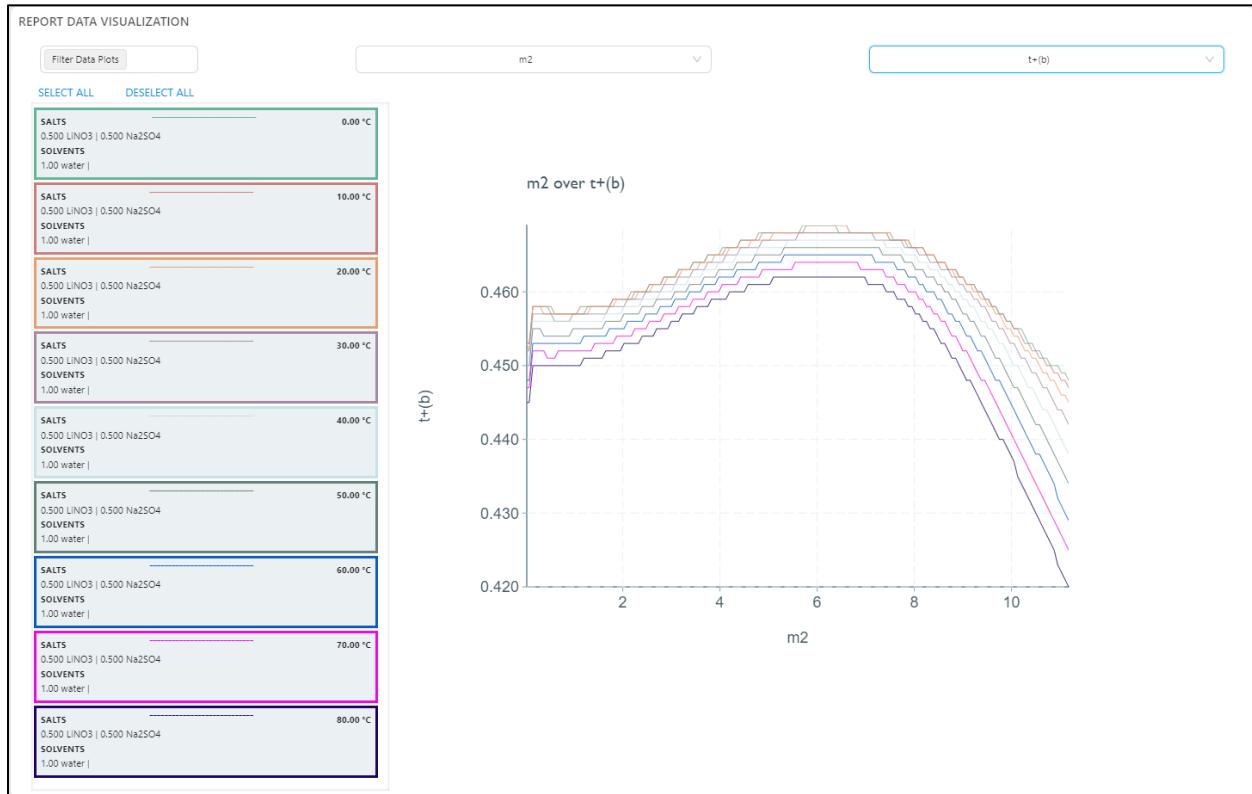


**Figure 101. Example 4 – Viscosity (cP) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)



**Figure 102. Example 4 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. ( $m_2$ ).**



**Figure 103. Example 4 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. ( $m_2$ ).**

## 4.5 Example 5: Matrix Optimization of Electrolyte Formulation with 4 Solvent, 2 Salt System

This example demonstrates a use case that performs optimization of a multi-solvent and dual salt electrolyte in terms of preferred solvent formulations and salt proportions. Optimization is done over ( $C_{\text{salt}}$ , T), allowing the user to have high-fidelity information that supports fine-tuning of the electrolyte according to anticipated conditions of the application. AEM large-scale optimization offers a means to screen millions of formulations and conditions to survey different property landscapes for the most promising combinations. This gives the AEM user a powerful research accelerator. Simulation inputs include the following:

- Four solvents (choose optimization) with PC, MP, BN, TMP. TMP will have a set mass fraction of 0.25
- Two-salt system with LiPF<sub>6</sub> and LiTFSI, using full matrix of salt proportions, up to 2.5 molal,
- T = 0°C to 50°C with 10°C steps,
- Use default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal
- No SCAEP; No DL.

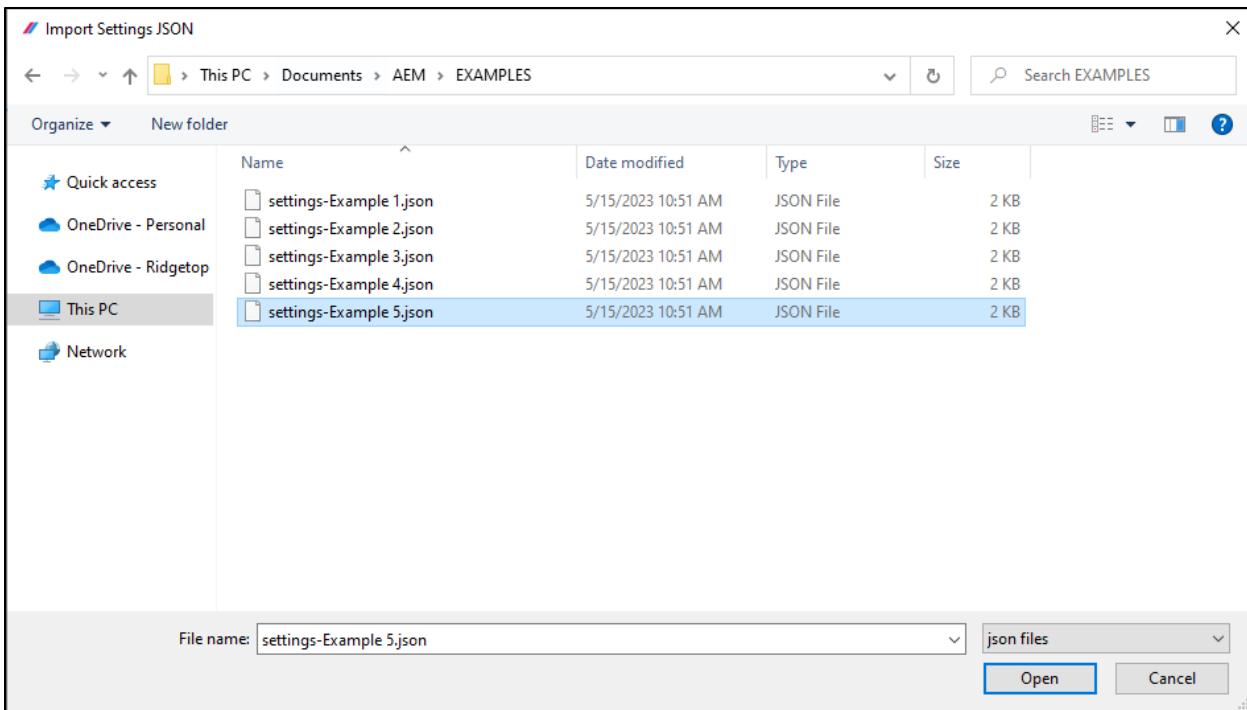
It should be noted that depending on input conditions, AEM optimization runs can take several minutes to hours depending on your computer setup. AEM optimization also produce large output files, some exceeding 1 GB in size. Upon run completion, Report07 contains an optimization summary.

### 4.5.1 Example 5: Importing Example 5 Parameters

We start off Example 5 by first using the **Import** Button from Section 3.5 to prepopulate each of the AEM input conditions for Example 5. This can be achieved by following the list of instructions below and referencing Figure 104 and Figure 105.

- a) Click on the **Import** (Import icon) Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- b) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- c) Select the **settings-Example 5.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 5.json" file was not imported successfully.



**Figure 104. Importing Example 5 Input Condition using the settings-Example 5.json file.**

### 4.5.2 Example 5: Overview of Simulation Input Conditions

Based on the conditions mentioned at the beginning of this example, select the following

- Select the four solvents PC, MP, BN, TMP. Choose optimization, where TMP has a set mass fraction of 0.25. As such, the software will determine optimal proportions of PC, MP and BN in relation to the set TMP fraction.
- Specify a two-salt system with LiPF<sub>6</sub> and LiTFSI, using full matrix of salt proportions. Set maximum salt concentration to 2.5 molal. Optimization will also include the influence of the mixed salt proportions,
- Select T = 0°C to 50°C with 10°C steps,
- Use default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal
- Choose No SCAEP; No DL.

**Important Note:** This example can take several minutes to hours to complete depending on your computational hardware. Please wait for the simulation to complete and then compare your data outputs in the discussion section.

## Advanced Electrolyte Model (AEM)

**Figure 105. Example 5 – AEM Input tab.**

### 4.5.3 Example 5: Data Output & Discussion

It is estimated that nearly 15,000 unique formulations were surveyed in this optimization run, each run over other matrices involving 7 temperatures and about 50 salt concentrations. That totals to about 5.25M total conditions. Any number of duplicate conditions are in addition to this number. Because these types of data output reports are so large and can be several GB in size, the AEM GUI has a built-in file size limit of 500MB. Any reports larger than that will not be automatically parsed to visualize the output graphs as shown in Examples 1-4.

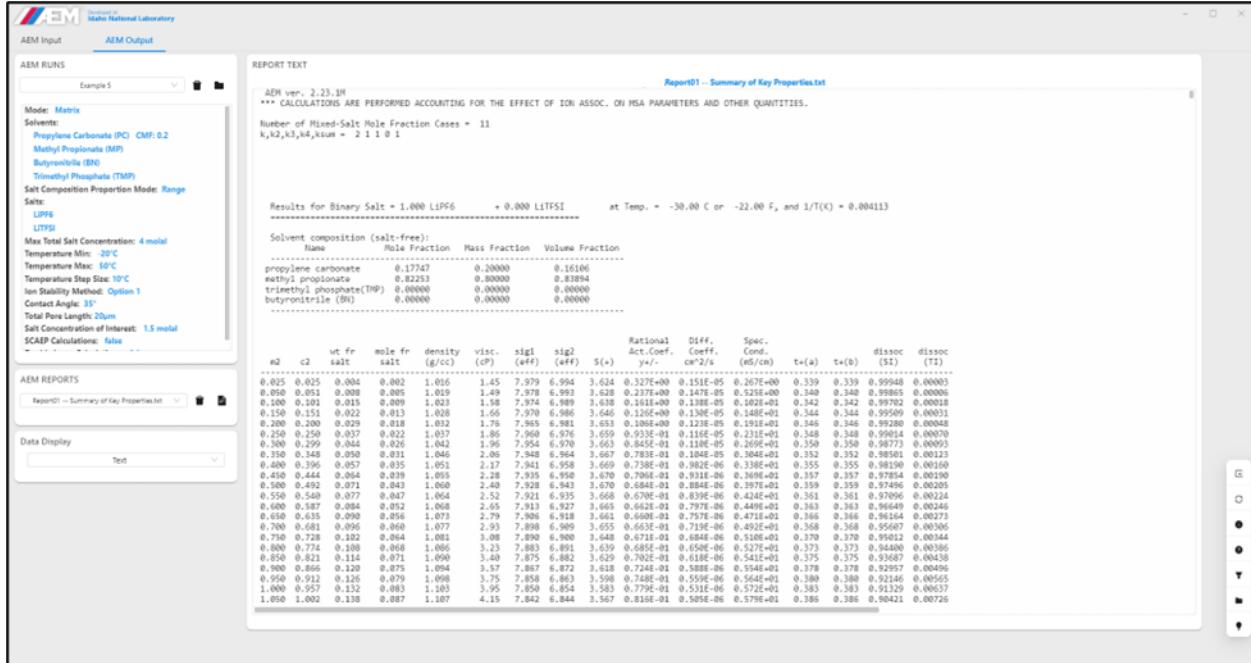
For this Example, Report07 contains an optimization results summary toward the end, where an assortment of optimization parameters is considered. The optimization outcomes can vary according to the target. For example, optimization in terms of conductivity over particular ( $C_{salt}$ ,  $T$ ) may yield a different general result than that for diffusivity and may differ as well from that obtained for the molecular-based process of cation desolvation (i.e., Li-STEP terms).

Results from Report07 indicate that low-to-no PC is preferred for transport properties such as conductivity and diffusivity, while higher amounts of BN are noted (about 56% by mass). This is due to how the presence of PC increases the solution viscosity. However, for considerations of cation desolvation (see optimization metrics tied to Li-STEP, Lithium Solvation and Transport Electrolyte Parameter), a low amount of BN is preferred, with a clear preference for optimizing

## Advanced Electrolyte Model (AEM)

around MP and TMP. This is generally due to how nitriles are aggressive solvators of cation species, and the relatively high cation solvation number that is obtained with PC. In some cases, the amount of desirable PC increases at higher salt levels, possibly due to the higher relative permittivity of PC that allows greater dissociation of salt.

Regarding the preferred amount of each salt, greater proportions of LiTFSI are noted for conductivity at relatively low salt concentrations, while the preference switches toward having more LiPF<sub>6</sub> for the diffusion coefficient, as well as for cation desolvation terms.



**Figure 106. Example 5 – AEM Output tab – REPORT TEXT section to view Report01–Report20.**

## 4.6 Example 6: ACCC Simulation with one ACCC Salt Definition

This example considers the two-solvent system from the ACCC Solvents EC\_EMC at a fixed volume fraction composition (30:70 vol %) with ACCC salt class as LiPF<sub>6</sub>\_w\_EC\_EMC. The salt concentration is allowed to go to 5 molal. Other factors behind the simulation include:

- T = -40°C to 60°C with 5°C steps,
- Used default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20μm, salt conc. of interest = 1.5 molal,
- No SCAEP; No DL.

The parameters for electrolyte ingress are relevant estimations for battery electrode materials in general and can be updated to reflect more finely tuned attributes of the porous media.

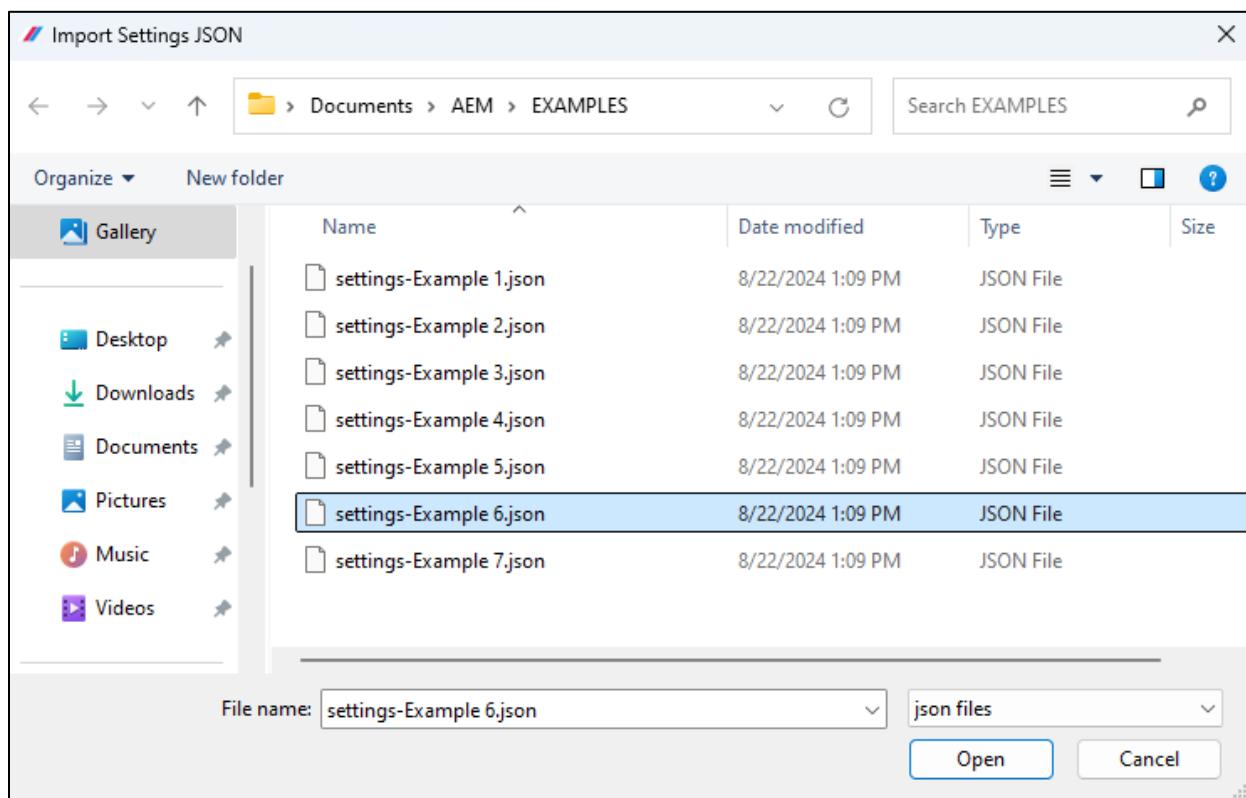
This relatively simple electrolyte represents a lower-viscosity, higher-conductivity system that would facilitate higher current densities in lithium-ion type cells. This electrolyte system has benefits toward conditions like moderately-fast charging and higher-power applications.

### 4.6.1 Example 6: Importing Example 6 Parameters

We start off Example 6 by first using the **Import** Button from Section 3.5 to prepopulate each of the AEM input conditions for Example 6. This can be achieved by following the list of instructions below and referencing Figure 107 and Figure 108.

- a) Click on the **Import** () Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- b) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- c) Select the **settings-Example 6.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 6.json" file was not imported successfully.



**Figure 107. Importing Example 6 Input Condition using the settings-Example 6.json file.**

### 4.6.2 Example 6: Overview of Simulation Input Conditions

Based on the conditions mentioned at the beginning of this example, select the following

- Select the EC\_EMC from the ACCC SOVENTS module. Provide 30:70 volume %
- Specify salt from the ACCC SALTS module as LiPF<sub>6</sub>\_w\_EC\_EMC. Set maximum salt concentration to 5 molal.
- T = -40°C to 60°C with 5°C steps,
- Choose default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35° , Pore length = 20μm, salt conc. of interest = 1.5 molal,
- Choose No SCAEP; No DL.

The screenshot shows the AEM software interface with the following settings:

- SINGLE FIXED COMPOSITION OF SOLVENTS**: Shows a 3x3 grid icon. Under "SELECT SOLVENTS", it lists "ACCC / EC\_EMC / ethylene carbonate" at 30% and "ACCC / EC\_EMC / ethylmethyl carbonate" at 70%.
- LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION**: Shows a 3x3 grid icon.
- TEMPERATURE SETTINGS**: Temperature Min: -30 °C, Temperature Max: 60 °C, Temperature Step Size: 5 °C to 10 °C.
- METHOD FOR HANDLING TRIPLE ION STABILITY**: Shows two inequalities:  $[ABA^+] = [BAB^-]$  (default) and  $[ABA^+] > [BAB^-]$  due to  $BAB^- + B^+ \leftrightarrow AB$  or  $[ABA^+] < [BAB^-]$  due to  $ABA^+ + A^+ \leftrightarrow AB$ . Inequalities are automatically determined.
- ELECTROLYTE INGRESS INTO PORES**: Contact Angle: 35°, Total Pore Length: 20 μm, Salt Concentration of Interest: 1.5 molal.
- SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP)**: Perform SCAEP Calculations:
- DOUBLE LAYER (DL)**: Perform DL Calculations:
- AEM RUN IDENTIFIER (optional)**: Run Identifier: Example 6, Append Timestamp:

At the bottom, there are buttons for "Run AEM" and "Append Multiple Runs".

**Figure 108. Example 6 – AEM Input tab.**

### 4.6.3 Example 6: Data Output & Discussion

Simulation outputs are plotted in Figure 110 - Figure 114 for the transport suite of properties (salt diffusivity, conductivity, viscosity, cation transference number). General goals for battery electrolytes are to achieve high diffusivity and conductivity, low viscosity and high cation transference. Since most property metrics exhibit a strong reliance on salt concentration, an effort should be made to identify the range of salt concentration that maximizes the foremost properties

## Advanced Electrolyte Model (AEM)

of interest. Note that this range should also consider the possible concentration polarization (CP) that can occur over more prolonged cycling elements, since CP will cause a salt depletion at one electrode, while causing an enrichment at the opposite electrode. Given these factors in concert, a feasible overall operational salt concentration range could be defined as 0.5 to 2.0 molal. Note that the effective temperature range for this example is -40 to 70 °C, since AEM adds temperature steps to enable calculation of activation energies over the user-specified range. Also note that for the cation transference values (Report01), the following is given:

(a) t+ evaluated with single-ion cations vs all charged species,

(b) t+ evaluated with all cation-bearing charged species vs all charged species.

The trends seen over these two approaches are very similar, where their behavior over salt concentration reflect the relative change in the local solvating structure around the lithium cations in relation to that of the anions.

**AEM RUNS**

Example 6-20240710\_150114

Mode: Fixed  
Solvent Comp. Proportionality Basis: Volume  
Solvents:  
EC\_EMC (ACCC) / ethylene carbonate Volume: 30  
EC\_EMC (ACCC) / ethylmethyl carbonate Volume: 70  
Salts:  
LiPF6\_w\_EC\_EMC (ACCO) / LiPF6  
Max Total Salt Concentration: 5 molal  
Temperature Min: -30°C  
Temperature Max: 60°C  
Temperature Step Size: 5°C  
Ion Stability Method: Option 1  
Contact Angle: 35°  
Iodide Ion Length: 20pm  
Salt Concentration of Interest: 1.5 molal  
SCAP Calculations: false  
Double Layer Calculations: false

**REPORT TEXT**

AEM ver. 2.24.2H-D-ACC  
\*\*\* CALCULATIONS ARE PERFORMED ACCOUNTING FOR THE EFFECT OF ION ASSOC. ON MSA PARAMETERS AND OTHER QUANTITIES.

Number of Mixed-Salt Mole Fraction Cases = 1  
k,k2,k3,k4,ksum = 1 0 0 0 1

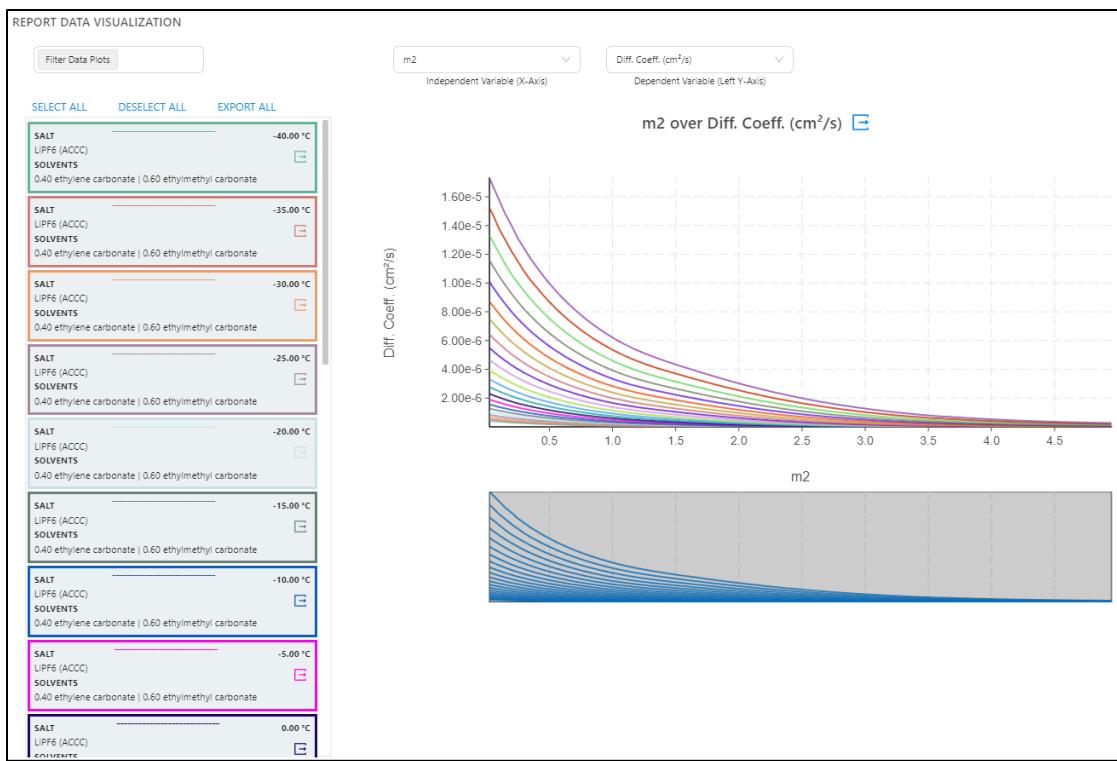
**Results for salt = LiPF6** (ACCC) at Temp. = -40.00 C or -40.00 F, and 1/T(K) = 0.004289

Solvent composition (salt-free):							
Name	Mole Fraction	Mass Fraction	Volume Fraction	Rational Act.Coeff.	Diff. Coeff.	Spec. Cond.	ye-/cm <sup>2</sup> /s
ethylene carbonate	0.40206	0.36255	0.30338	(ACCC)			
ethylmethyl carbonate	0.59794	0.63745	0.69662	(ACCC)			

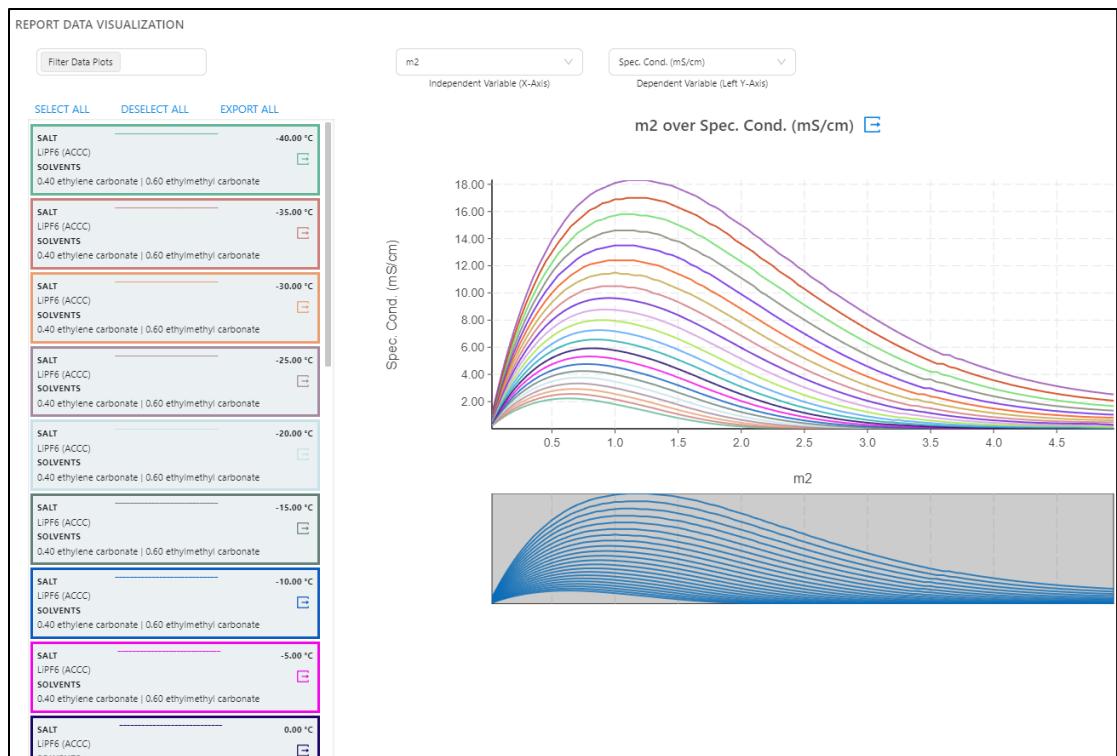
m2	c2 <sub>eff</sub>	wt fr	mole fr	density	visc.	sig1 (eff)	sig2 (eff)	5(+)	Rational Act.Coeff.	Diff. Coeff.	Spec. Cond.	t+(a)	t+(b)	dissoc (SI)	dissoc (TI)	
m2	c2 <sub>trans</sub>	salt	salt	(g/cc)	(CP)				ye/-	cm <sup>2</sup> /s	(m <sup>2</sup> /cm)					
0.025	0.029	0.028	0.004	1.79	1.63	8.231	7.710	3.832	0.645E+00	0.415E-05	0.200E+00	0.439	0.439	0.99997	0.00000	
0.050	0.059	0.059	0.008	0.805	1.181	3.81	8.231	7.710	3.844	0.592E+00	0.396E-05	0.402E+00	0.440	0.440	0.99998	0.00000
0.100	0.117	0.117	0.015	0.010	1.186	4.17	8.226	7.711	3.868	0.550E+00	0.368E-05	0.748E+00	0.442	0.442	0.99972	0.00001
0.150	0.175	0.175	0.022	0.014	1.191	4.56	8.226	7.704	3.889	0.540E+00	0.328E-05	0.105E+01	0.444	0.444	0.99949	0.00002
0.200	0.233	0.233	0.029	0.019	1.196	4.98	8.213	7.697	3.908	0.547E+00	0.308E-05	0.130E+01	0.446	0.446	0.99917	0.00004
0.250	0.269	0.269	0.036	0.020	1.202	5.32	8.205	7.690	3.929	0.539E+00	0.280E-05	0.156E+01	0.448	0.448	0.99877	0.00008
0.300	0.346	0.345	0.044	0.028	1.205	5.90	8.198	7.680	3.942	0.525E-06	0.171E+01	0.449	0.449	0.99824	0.00015	
0.350	0.402	0.401	0.050	0.033	1.213	6.42	8.189	7.670	3.956	0.626E+00	0.231E-06	0.186E+01	0.451	0.451	0.99756	0.00026
0.400	0.450	0.457	0.057	0.038	1.215	6.98	8.181	7.659	3.968	0.671E+00	0.212E-06	0.199E+01	0.453	0.453	0.99665	0.00045
0.450	0.514	0.512	0.064	0.042	1.219	7.59	8.172	7.648	3.978	0.728E+00	0.195E-06	0.205E+01	0.454	0.454	0.99552	0.00074
0.500	0.569	0.566	0.070	0.047	1.221	8.07	8.163	7.636	3.989	0.786E+00	0.179E-06	0.218E+01	0.455	0.455	0.99418	0.00119
0.550	0.623	0.620	0.077	0.051	1.228	9.02	8.153	7.625	3.991	0.880E+00	0.164E-06	0.221E+01	0.457	0.457	0.99237	0.00187
0.600	0.670	0.672	0.088	0.055	1.233	9.85	8.143	7.613	3.994	0.981E+00	0.150E-06	0.223E+01	0.459	0.459	0.99003	0.00290
0.650	0.732	0.725	0.090	0.060	1.237	10.79	8.133	7.601	3.994	0.110E+01	0.137E-06	0.223E+01	0.460	0.461	0.98703	0.00443
0.700	0.776	0.776	0.098	0.064	1.241	11.84	8.123	7.589	3.998	0.125E-06	0.125E-06	0.461	0.461	0.98395	0.00668	
0.750	0.839	0.832	0.102	0.066	1.246	13.04	8.114	7.576	4.002	0.143E+01	0.114E-06	0.216E+01	0.462	0.462	0.98059	0.00959
0.800	0.892	0.876	0.108	0.072	1.251	14.34	8.103	7.564	3.972	0.164E+01	0.103E-06	0.213E+01	0.463	0.466	0.97233	0.01402
0.850	0.945	0.925	0.116	0.077	1.255	15.83	8.093	7.552	3.958	0.190E+01	0.934E-07	0.206E+01	0.464	0.467	0.95656	0.01933
0.900	0.997	0.972	0.120	0.081	1.259	17.50	8.083	7.540	3.939	0.222E+01	0.846E-07	0.198E+01	0.465	0.469	0.95683	0.02663
0.950	1.041	1.018	0.126	0.085	1.264	19.34	8.073	7.528	3.904	0.256E+01	0.766E-07	0.196E+01	0.467	0.470	0.94588	0.03604
1.000	1.084	1.061	0.132	0.089	1.268	21.39	8.062	7.507	3.869	0.294E+01	0.694E-07	0.194E+01	0.468	0.473	0.93722	0.04763
1.050	1.132	1.104	0.138	0.093	1.272	23.61	8.051	7.508	3.849	0.353E+01	0.628E-07	0.171E+01	0.464	0.473	0.91687	0.06191
1.100	1.203	1.144	0.143	0.097	1.277	26.04	8.041	7.498	3.800	0.414E+01	0.570E-07	0.161E+01	0.463	0.475	0.89883	0.07835
1.150	1.254	1.183	0.149	0.101	1.281	28.71	8.036	7.490	3.756	0.486E+01	0.517E-07	0.151E+01	0.461	0.476	0.87923	0.09628
1.200	1.304	1.220	0.154	0.105	1.285	31.75	8.019	7.482	3.711	0.573E+01	0.468E-07	0.141E+01	0.459	0.477	0.85953	0.11424

**Figure 109. Example 6 – AEM Output tab – REPORT TEXT section to view Report01-Report20.**

## Advanced Electrolyte Model (AEM)

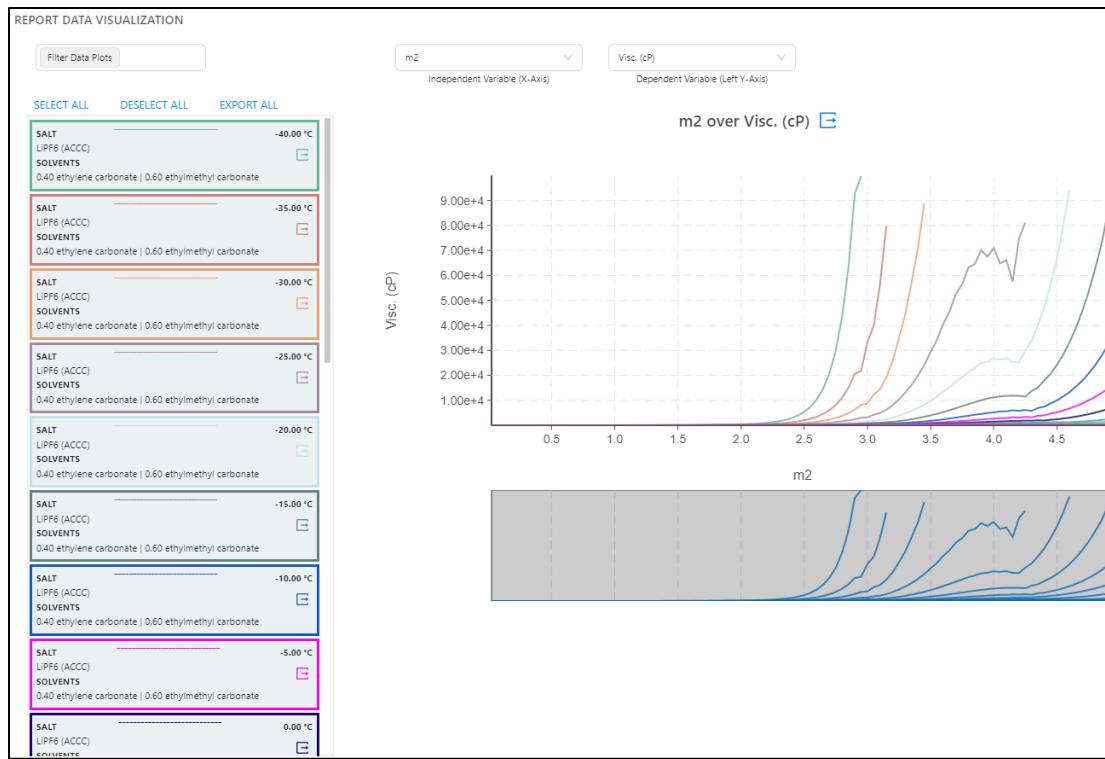


**Figure 110. Example 6 – Diffusivity/Diffusion Coefficient (cm<sup>2</sup>/s) v/s Molal Salt Conc. (m<sup>2</sup>).**

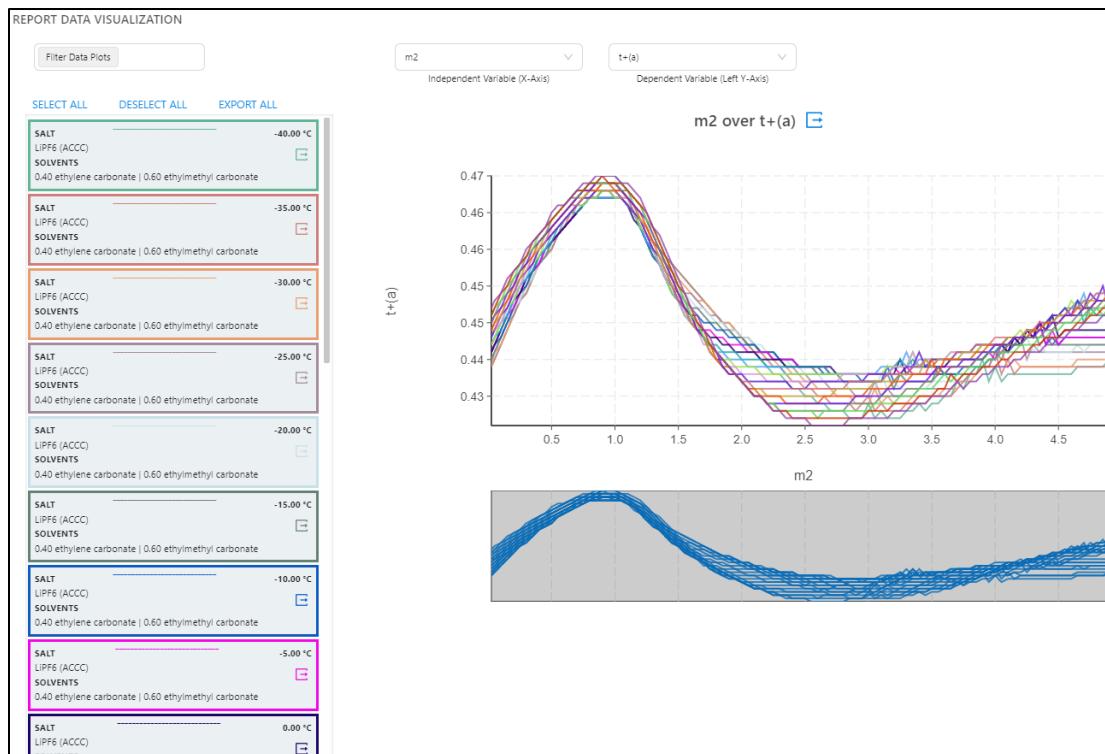


**Figure 111. Example 6 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m<sup>2</sup>).**

## Advanced Electrolyte Model (AEM)

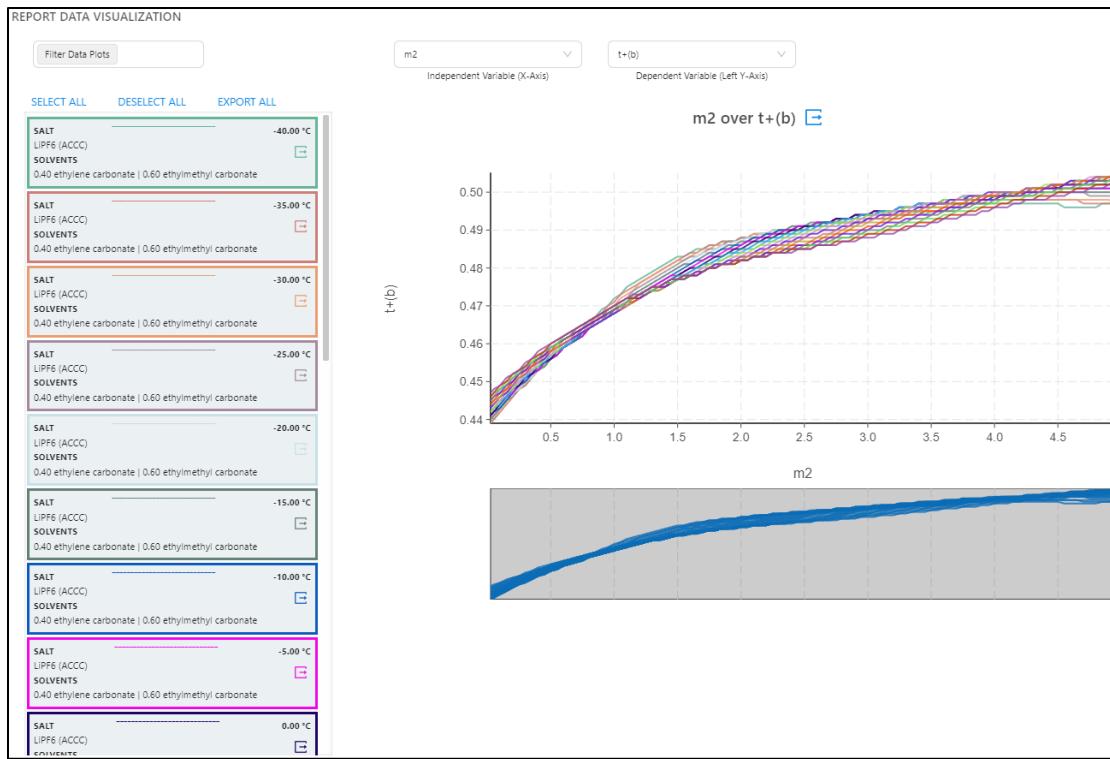


**Figure 112. Example 6 – Viscosity (cP) v/s Molal Salt Conc. (m2).**



**Figure 113. Example 6 – Cation Transference No. (t+(a)) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)



**Figure 114. Example 6 – Cation Transference No. ( $t+(b)$ ) v/s Molal Salt Conc. ( $m_2$ ).**

## 4.7 Example 7: Two Salt Simulation with one Default Library Salt and one ACCC Salt

This example considers the two-salt system. One salt from the ACCC Salt class LiBOB\_w\_PC\_EA and the second one from the default library LiPF6 at a fixed molar proportion (50:50). The salt concentration is allowed to go to 3 molal. Other factors behind the simulation include:

- T = -20°C to 50°C with 5°C steps,
- Used default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal,
- No SCAEP; No DL.

The parameters for electrolyte ingress are relevant estimations for battery electrode materials in general and can be updated to reflect more finely tuned attributes of the porous media.

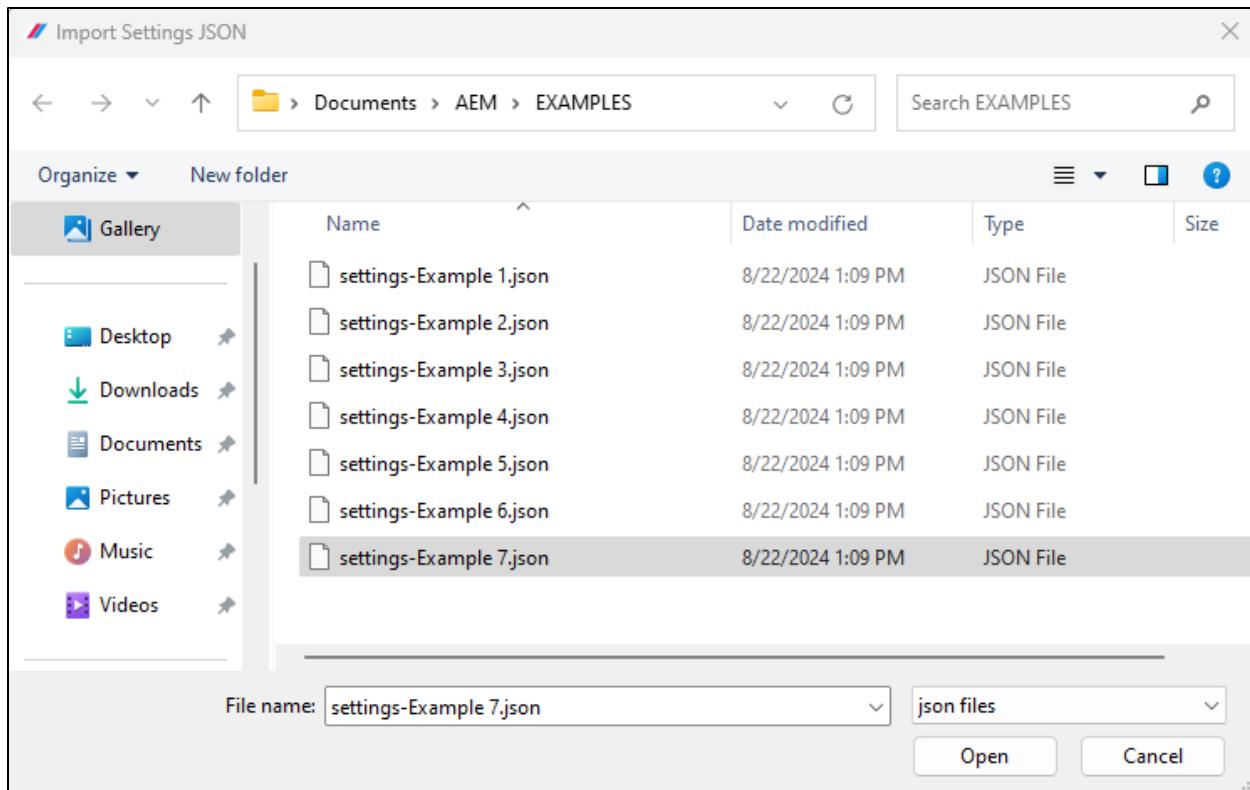
This relatively simple electrolyte represents a lower-viscosity, higher-conductivity system that would facilitate higher current densities in lithium-ion type cells. This electrolyte system has benefits toward conditions like moderately-fast charging and higher-power applications.

### 4.7.1 Example 7: Importing Example 7 Parameters

We start off Example 7 by first using the **Import** Button from Section 3.5 to prepopulate each of the AEM input conditions for Example 7. This can be achieved by following the list of instructions below and referencing Figure 115 and Figure 116.

- d) Click on the **Import** (Import icon) Button in the **Global Features & Icons** section in the lower left corner of the GUI.
- e) Verify that the GUI prompts to the **C:\Users\user-name\Documents\AEM\EXAMPLES\** directory in Windows File Explorer.
- f) Select the **settings-Example 7.json** file and click the **Open** button.

**Important Note:** An error message will pop up if the "settings-Example 7.json" file was not imported successfully.



**Figure 115. Importing Example 7 Input Condition using the settings-Example 7.json file.**

#### 4.7.2 Example 7: Overview of Simulation Input Conditions

Based on the conditions mentioned at the beginning of this example, select the following

- Select a single solvent PC from the default solvent library.
- Select the two salts, LiBOB\_w\_PC\_EA from the ACCC salt class and LiPF6 from the default salt class with 50:50 molar proportion. Set maximum salt concentration to 3 molal,
- Select T = -20°C to 50°C with 10°C steps,
- Use default method for handling triple ion stability,
- Inputs for electrolyte ingress into pores: contact angle = 35°, Pore length = 20µm, salt conc. of interest = 1.5 molal
- Choose No SCAEP; No DL.

## Advanced Electrolyte Model (AEM)

**Figure 116. Example 7 – AEM Input tab.**

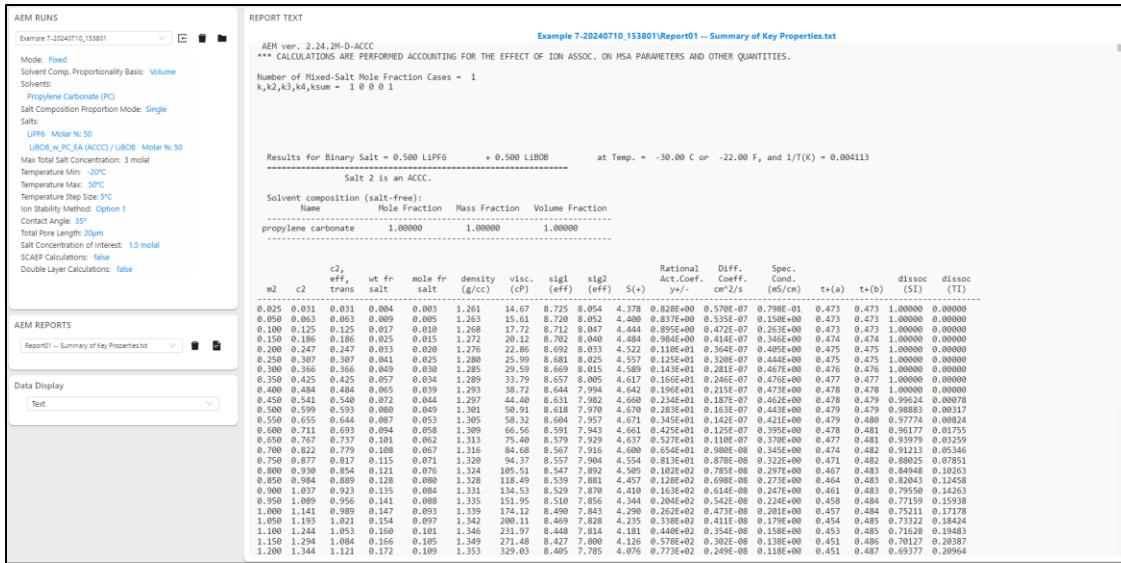
### 4.7.3 Example 7: Data Output & Discussion

Simulation outputs are plotted in Figure 118 – Figure 122 for the transport suite of properties (salt diffusivity, conductivity, viscosity, cation transference number). General goals for battery electrolytes are to achieve high diffusivity and conductivity, low viscosity and high cation transference. Since most property metrics exhibit a strong reliance on salt concentration, an effort should be made to identify the range of salt concentration that maximizes the foremost properties of interest. Note that this range should also consider the possible concentration polarization (CP) that can occur over more prolonged cycling elements, since CP will cause a salt depletion at one electrode, while causing an enrichment at the opposite electrode. Note that the effective temperature range for this example is -30 to 55 °C, since AEM adds temperature steps to enable calculation of activation energies over the user-specified range. Also note that for the cation transference values (Report01), the following is given:

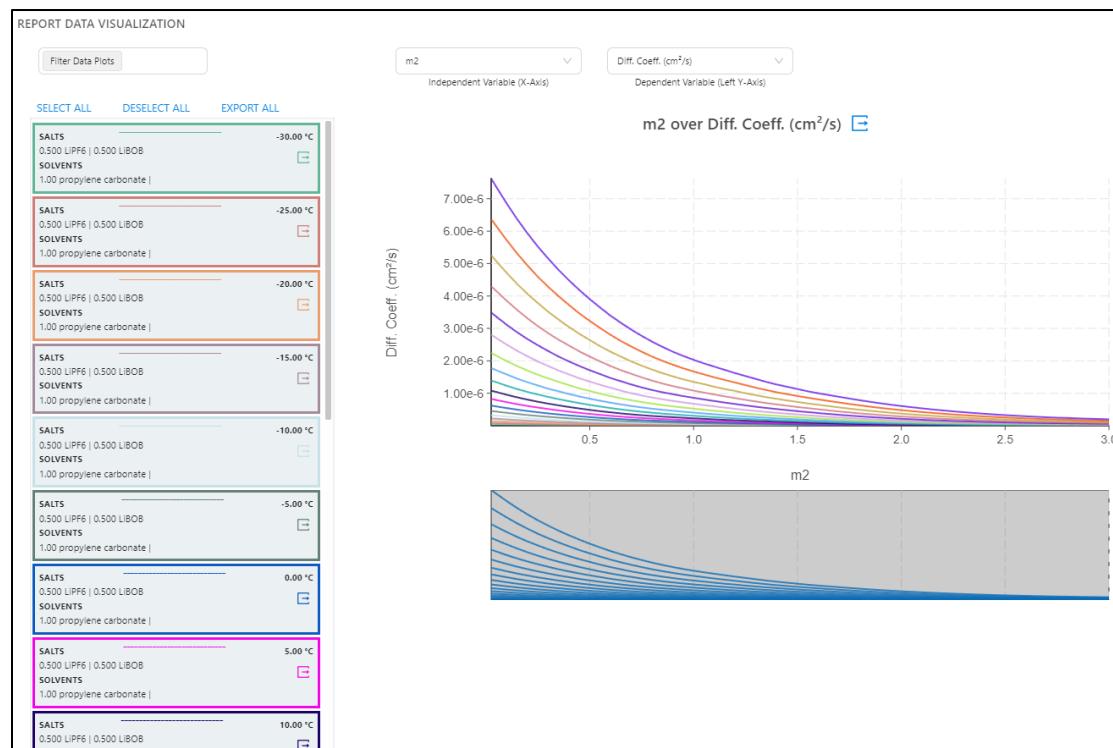
- (a) t+ evaluated with single-ion cations vs all charged species,
- (b) t+ evaluated with all cation-bearing charged species vs all charged species.

The trends seen over these two approaches are very similar, where their behavior over salt concentration reflect the relative change in the local solvating structure around the lithium cations in relation to that of the anions.

## Advanced Electrolyte Model (AEM)

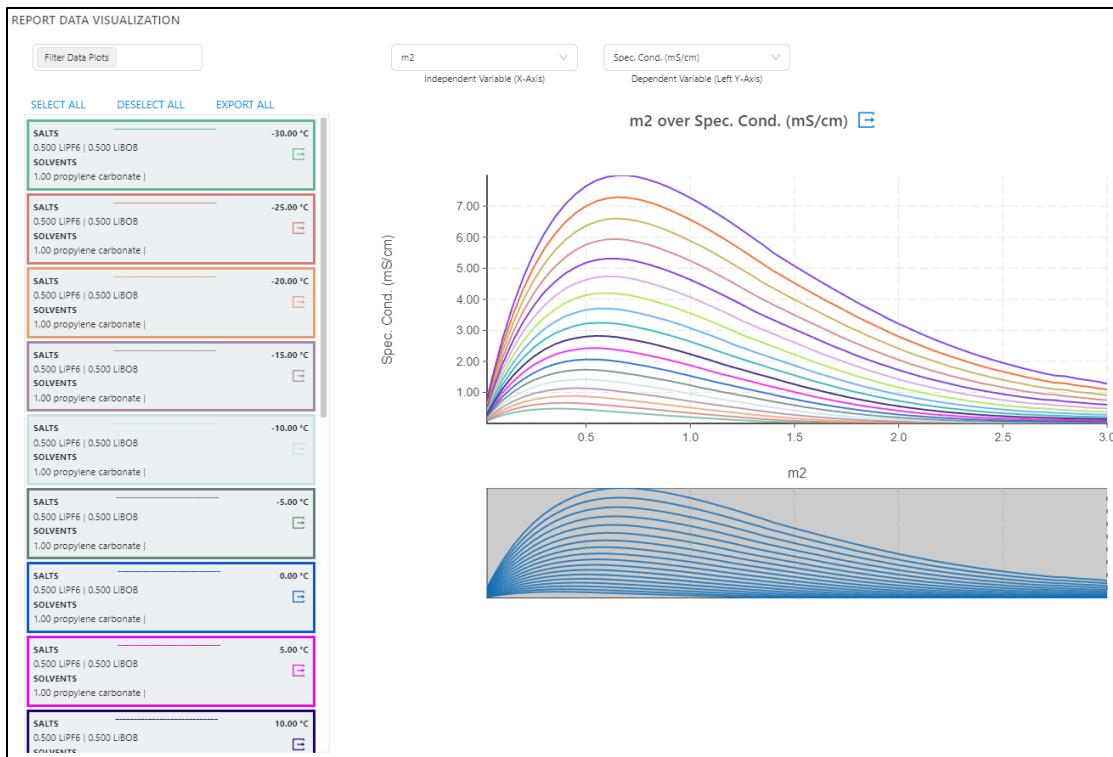


**Figure 117. Example 7 - AEM Output tab – REPORT TEXT section to view Report01–Report20.**

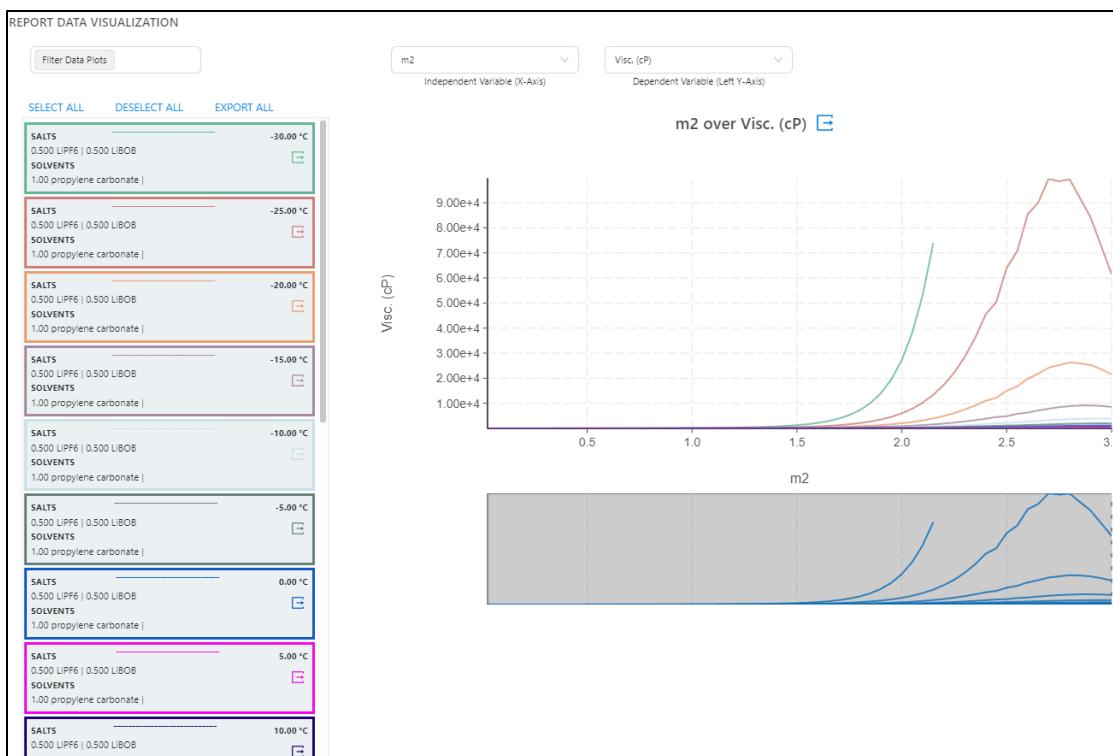


**Figure 118. Example 7 – Diffusivity/Diffusion Coefficient (cm<sup>2</sup>/s) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)

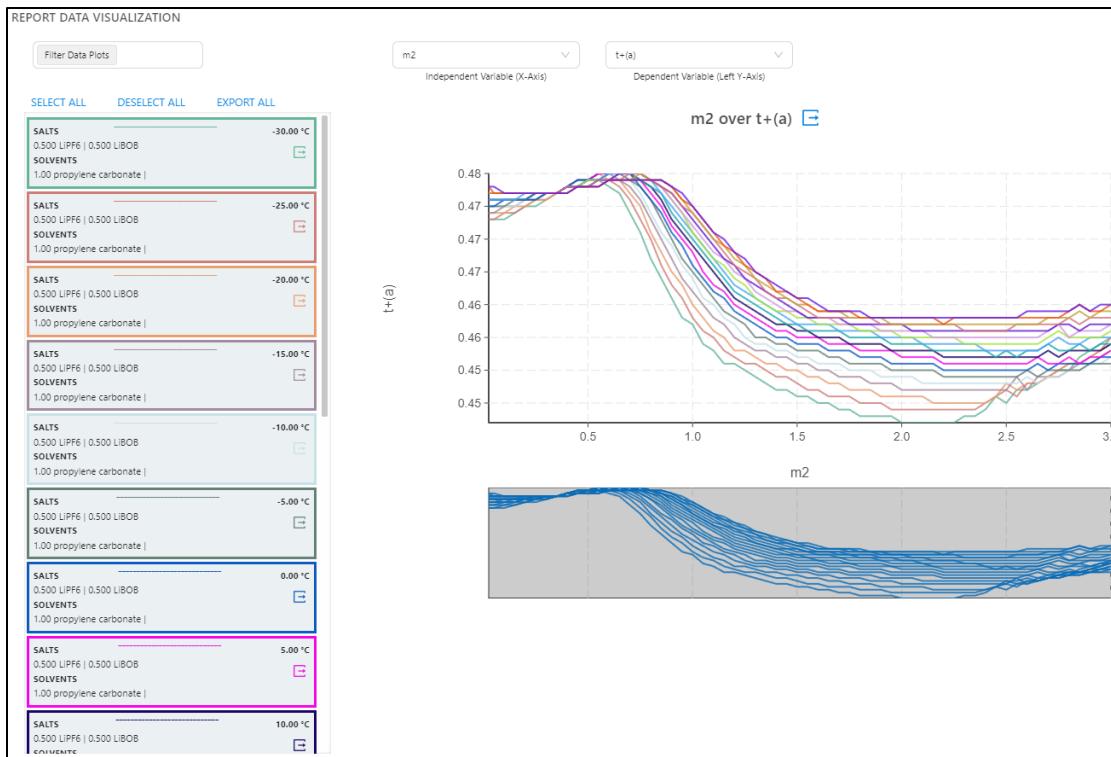


**Figure 119. Example 7 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).**

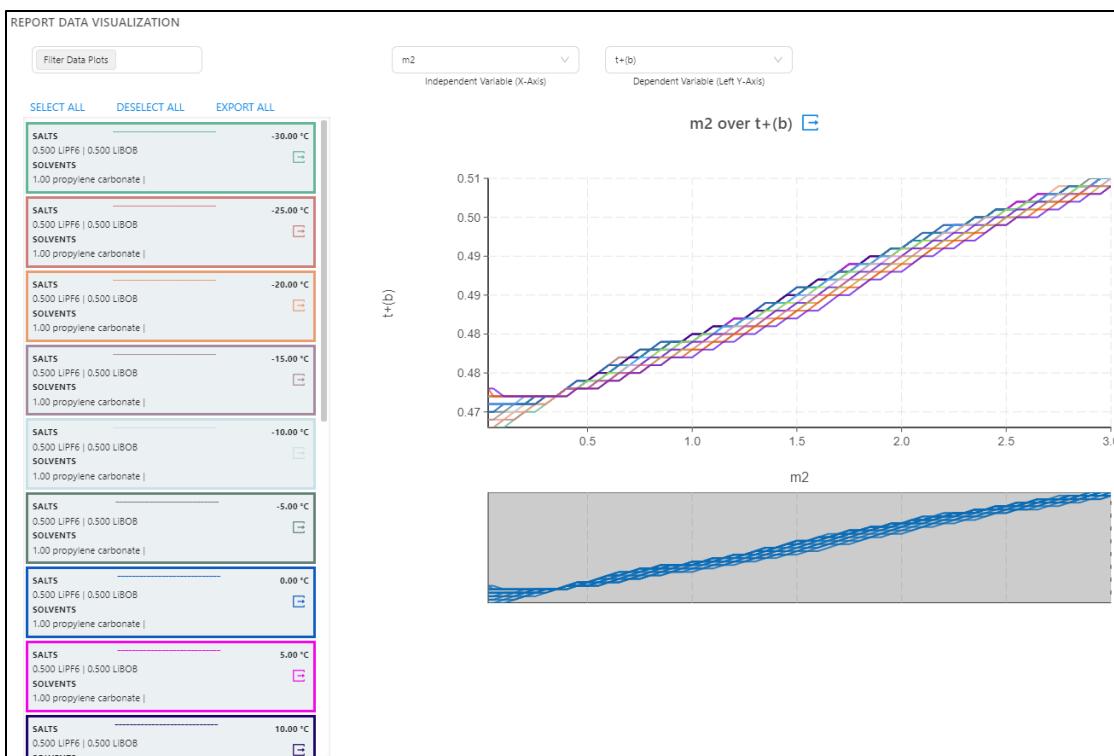


**Figure 120. Example 7 – Viscosity (cP) v/s Molal Salt Conc. (m2).**

## Advanced Electrolyte Model (AEM)



**Figure 121. Example 7 – Cation Transference No. ( $t+(a)$ ) v/s Molal Salt Conc. ( $m_2$ ).**



**Figure 122. Example 7 – Cation Transference No. ( $t+(b)$ ) v/s Molal Salt Conc. ( $m_2$ ).**

## 5 AEM Command Line Interface (CLI)

### 5.1 AEM CLI Overview

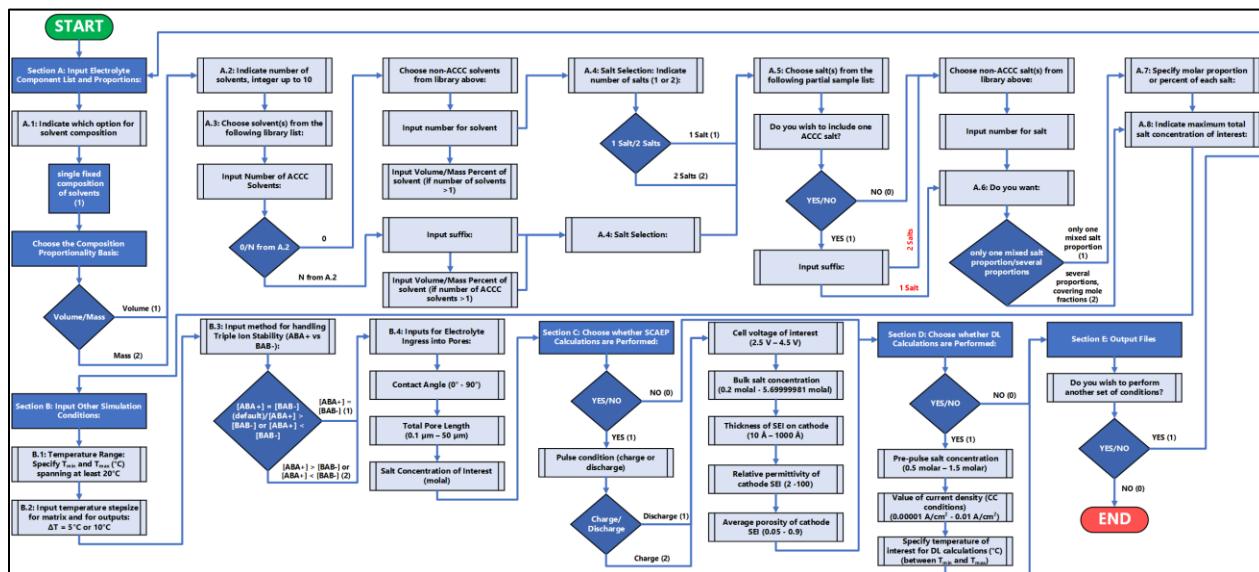
The AEM Graphical User Interface (GUI) covered in Section 3 and Section 4, utilizes the original AEM Command Line Interface (CLI) executable program. Within both AEM programs, the software is organized based on the composition of the substituents that go in the user's desired electrolyte as well as other key simulation conditions.

For the AEM CLI program there are six sections of settings: A. Input Electrolyte Component List and Proportions, B. Input Other Simulation Conditions, C. Choose whether Surface-Charge Attenuated Electrolyte Permittivity (SCAEP) Calculations are Performed, D. Choose whether Double Layer (DL) Calculations are Performed, and E. Output Files.

**Important Note:** The traditional AEM CLI program is not available in the AEM Trial Version of the software. Contact Ridgetop Group or INL directly if you wish to upgrade to the full product version of AEM.

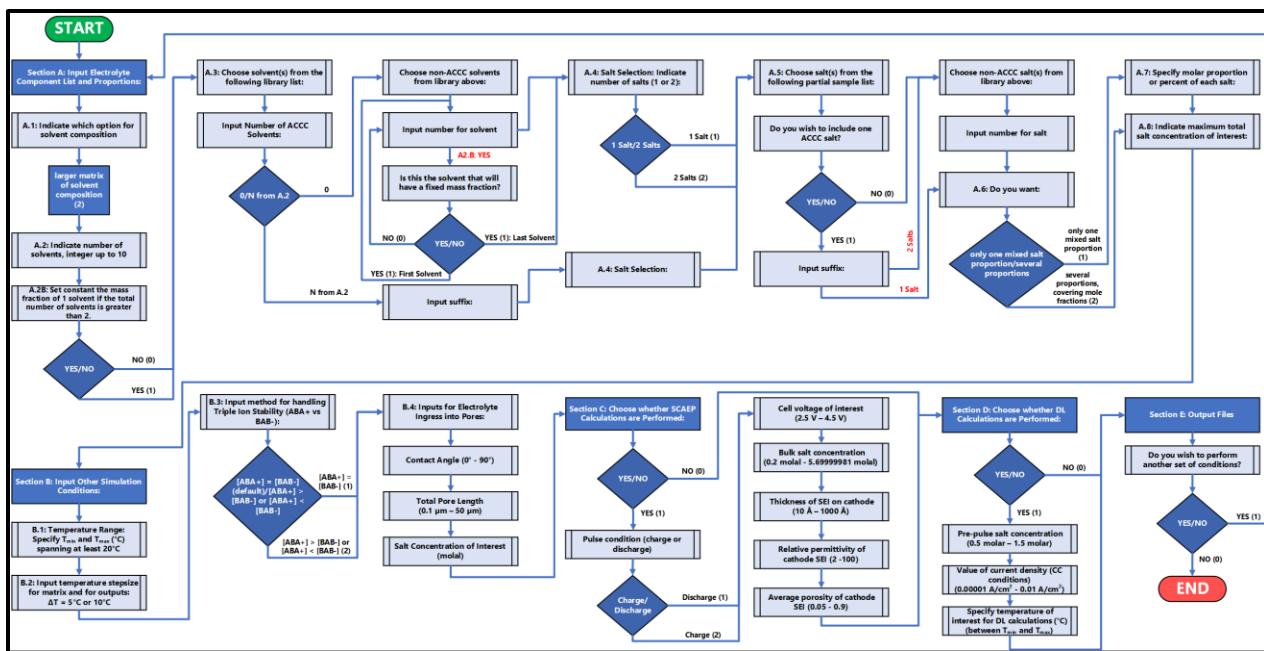
### 5.2 AEM CLI Program Flow Chart

The overall program flow follows the path shown in Figure 123 and Figure 124 below, based on what solvent composition is used. AEM starts by offering the option to run with minimal interaction from the operator or user. The other option is to run interactively where the operator or user supplies simulation conditions.



**Figure 123. AEM Fortran Version 2.24.2 Program Flow – single fixed composition of solvents is chosen in A.1.**

## Advanced Electrolyte Model (AEM)



**Figure 124. AEM Fortran Version 2.24.2 Program Flow – larger matrix of solvent composition is chosen in A.1.**

## 5.3 Running Example 1 with AEM CLI

**Important Note:** This section only describes running Example 1 with the AEM CLI. The user can simulate other examples by following the process outlined for Example 1. If further technical support or guidance is needed, contact a Ridgetop or INL representative directly.

### 5.3.1 Setup to Run Example 1 with AEM CLI

We start off Example 1 by first locating the AEM CLI executable in the AEM program directory. The executable file is named **aem-2242m-d-accc** and is in ...\\AEM\\CLI\\. A visual of this file is shown in Figure 125, but do note that “**2242**” corresponds to the AEM CLI version number and your version may be different. To execute AEM on the CLI, right click on the file and select **Open** or **Run as Administrator**, or alternatively **double-click it**. Next, verify that the command prompt opens with the following welcome message as shown in Figure 126.

## Advanced Electrolyte Model (AEM)

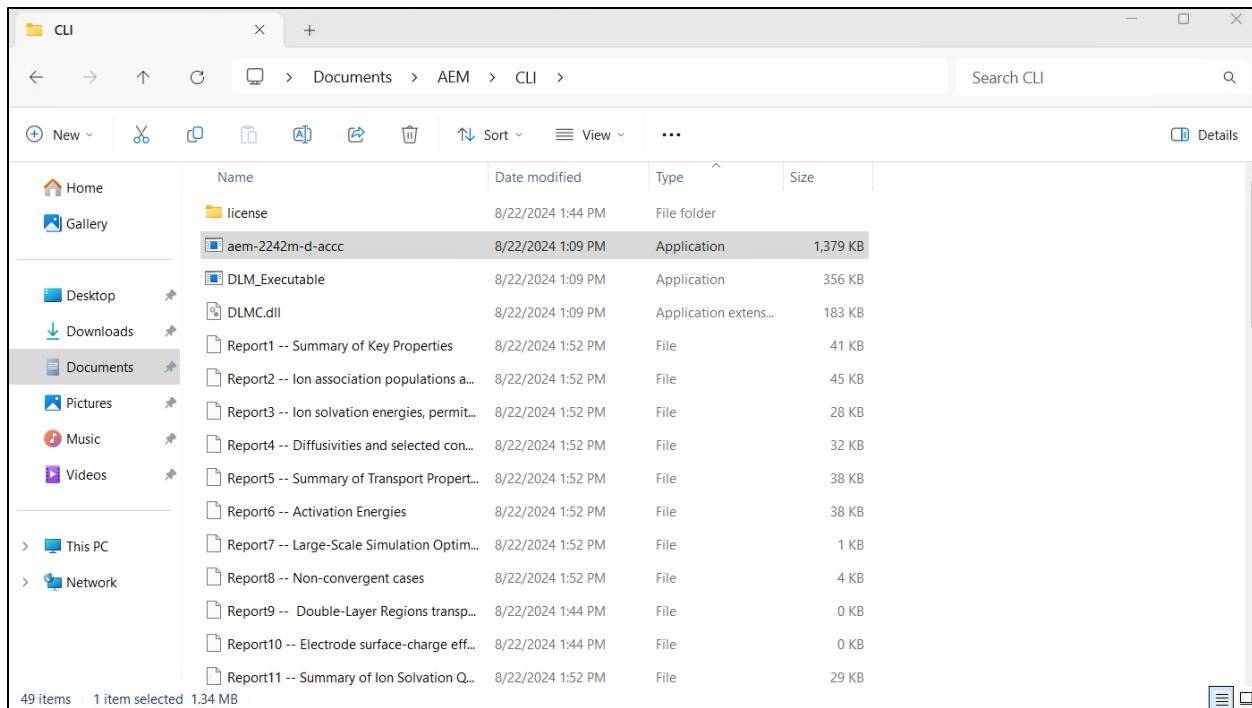


Figure 125. aem-2242m-d-accc CLI Executable in ...\\AEM\\CLI\\.

```
C:\Users\WDAGUtilityAccount\Documents\AEM\CLI\ aem-2242m-d-accc.exe

AEM: Welcome to Advanced Electrolyte Model, ver. 2.24.2M-D-ACCC

Created by Kevin L. Gering, PhD (INL)
Sponsored by U. S. Department of Energy and INL

Primary Application: Electrolytes for Li and Na-ion batteries

* Disclaimer: not all your choices of components
and conditions will produce viable electrolytes.

Section A: input electrolyte component list and proportions

A.1: Indicate which option for solvent composition:
Option 1: single fixed composition of solvents.
    --> Up to 10 solvents per formulation
Option 2: larger matrix of solvent composition
    for optimization of electrolyte formulation;
    matrix is at default setting.
    --> Up to 5 solvents in optimization
    (warning: can produce extensive output!)

Input 1 or 2:
```

Figure 126. Welcome Message prompt when AEM is first run.

### 5.3.2 Section A: Input Electrolyte Component List and Proportions:

This section defines the user's desired electrolyte's input components and their proportion. This section contains 6 subsections based on the user's desired qualitative and quantitative inputs.

#### A.1: Indicate which option for solvent composition:

This is where the user chooses from the two available options for solvent composition. As shown in Figure 127, for Example 1, we use **Option 1: single fixed composition of solvents**. which will run a finite number of solvents to formulate the composition of the electrolyte.

```
A.1: Indicate which option for solvent composition:
    Option 1: single fixed composition of solvents.
                ---> Up to 10 solvents per formulation
    Option 2: larger matrix of solvent composition
                for optimization of electrolyte formulation;
                matrix is at default setting.
                ---> Up to 5 solvents in optimization
                (warning: can produce extensive output!)
```

**Input 1 or 2:**

**1**

**Figure 127. Section A.1 from AEM Fortran Version 2.24.2**

When **Option 1** is chosen, the program prompts the user to choose the composition proportionality basis as either **Volume** or **Mass**. As shown in Figure 128, for Example 1, we use **Volume** which will fix the volume proportions of our solvents to formulate the composition of the electrolyte.

```
For Option 1, choose the composition proportionality basis:
    1 = Volume
    2 = Mass

    Input 1 or 2:
        1
```

**Figure 128. Prompt to Input 1 for Section A.1 from AEM Fortran Version 2.24.2.**

#### A.2: Indicate number of solvents, integer up to 10:

This is where the user defines the number of solvents that are combined to formulate the desired electrolyte. The maximum number of solvents allowed as inputs to the program using **Option 1: single fixed composition of solvents**. is **ten (10)**. As shown in Figure 129, for Example 1, we use **three (3)** solvents.

**A.2: Indicate number of solvents, integer up to 10**  
**3**

Figure 129. Section A.2F from AEM Fortran Version 2.24.2.

**A.3: Choose solvent(s) from the following library list:**

This is where the user defines the type of solvent (based on existing chemistries in the AEM library) for each solvent specified in A.3. If applicable, this is also where the user can define how many ACCC Solvents are included in the simulation. As shown in Figure 130 and Figure 131, for Example 1, we do not include any ACCC solvents and use **3: ethylene carbonate (EC)**, **8: dimethyl carbonate (DMC)**, and **12: ethyl propionate (EP)**.

```
A.3: Choose solvent(s) from the following library list:

1: water

CARBONATES:
 2: propylene carbonate (PC)
 3: ethylene carbonate (EC)
 6: ethylmethyl carbonate (EMC)
 7: diethyl carbonate (DEC)
 8: dimethyl carbonate (DMC)
15: fluoroethylene carbonate (FEC)
39: vinylene carbonate (VC)
45: vinyl ethylene carbonate (VEC)

DICARBONATES:
 49: Dimethyl 2,5, Dioxahexanedioate (DMOHC)
 50: Diethyl 2,5, Dioxahexanedioate (DEOHC)

GLYMES
 5: 1,2-dimethoxyethane (DME)
 59: 1,2-dimethoxyp propane (DMP)
20: DEGOME (diglyme)
21: 3-TEGDME (triglyme)
22: 4-TEGDME (tetraglyme)

S or P CONTAINING SOLVENTS:
16: ethylmethoxyethyl sulfone (EMES)
28: ethylmethyl sulfone (EMS)
34: sulfolane (TMS)
35: trimethyl phosphate (TMP)
55: triethyl phosphate (TEP)
46: (proprietary, unavailable)
60: dimethyl sulfite (DMS)

FROM OTHER CLASSES:
 4: gamma-butyrolactone (GBL)
10: 1,3 dioxolane
14: ethylene glycol (EG)
17: Dowanol-PMA (DOW-PMA)
18: 2-methoxyethyl acetate (MEA)
19: 1NM2-siloxane (1NM2)
47: Tris(2,2,2-trifluoroethyl)-orthoformate (TFEO)
51: 7-oxabicyclo[2.2.1]heptane-2-carbonitrile (OCN)
52: tetrahydrofuran (THF)
53: (proprietary, unavailable)
54: (proprietary, unavailable)
56: Bis(2,2,2-trifluoroethyl) ether (BTFE)
57: 1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether (TTE)
63: Fluorobenzene (FBZ)

ESTERS:
 9: ethyl acetate (EA)
11: methyl butyrate (MB)
12: ethyl propionate (EP)
13: n-propyl acetate (nPA)
29: methyl acetate (MA)
30: methyl propionate (MP)
31: methyl formate (MF)
32: ethyl formate (EF)
37: methyl monofluoroacetate (M1FA)
38: methyl difluoroacetate (M2FA)
58: ethyl difluoroacetate (E2FA)
40: n-propyl propionate (nPP)
42: n-butyl acetate (nBA)
43: n-butyl propionate (nBP)
44: n-butyl butyrate (nBB)

NITRILES AND DINITRILES:
26: glutaronitrile (GLN)
27: adiponitrile (ADN)
33: propionitrile (PN)
36: acetonitrile (AN)
41: butyronitrile (BN)
48: succinonitrile (SN)
61: isovaleronitrile (IVN)
62: isobutyronitrile (IBN)

PHOSPHAZENE ADDITIVES:
23: INL Additive FM2
24: INL Additive SM4
25: INL Additive PA5
```

Figure 130. Section A.3 (1) from AEM Fortran Version 2.24.2.

```
--> You have an option to designate some solvents as Arbitrarily-Chosen  
Chemical Compounds (ACCC), which may or may not be listed in the solvent  
library above. ACCC parameters will be housed in and read from the file  
"ACCC Inputs (Solvent Class)--suffix"  
that you provide (input structure per K. Gering).
```

How many ACCC solvents are included in the overall solvent number?

Input Number of ACCC Solvents: 0 to 3

0

Choose non-ACCC solvents from library above:

Input number for solvent 1 :

3

Input number for solvent 2 :

8

Input number for solvent 3 :

12

**Figure 131. Selecting solvents in CLI Example 1.**

In this section, the CLI also prompts the user to select the volume percentages of the selected solvents. As shown in Figure 132, for Example 1, we use **25% EC**, **50% DMC**, and **25% EP**.

```
Input Volume Percent of solvent 1 :  
      25  
Input Volume Percent of solvent 2 :  
      50  
Input Volume Percent of solvent 3 :  
      25  
Percentage sums not equal to 100 will be derived by relative input proportions.
```

**Figure 132. Section A.3 (2) from AEM Fortran Version 2.24.2.**

**A.4: Indicate number of salts (1 or 2):**

This is where the user defines the number of salts used to formulate the desired electrolyte. The maximum number of salts allowed as inputs to the program is **two (2)**. As shown in Figure 133. For Example 1, we use **one (1)** salt.

**A .4 : Indicate number of salts (1 or 2)**

**Input 1 or 2:**

**1**

**Figure 133. Section A.4 from AEM Fortran Version 2.24.2.**

## Advanced Electrolyte Model (AEM)

### A.5: Choose salt(s) from the following partial sample list:

This is where the user defines the type of salt (based on existing chemistries in the AEM library) for each solvent specified in A.4. As shown in Figure 134, for Example 1, we do not include any ACCC salts and use 7: LiPF<sub>6</sub>.

```
A.5: Choose salt(s) from the following partial sample list:

    For Battery Electrolytes:
        7: LiPF6
        8: LiBF4
        9: LiBOB
        10: LiTFSI
        11: Li2(B12F12)
        12: LiDFOB
        38: LiDFBOP
        13: LiFSI
        14: Li-Triflate
        15: LiAsF6
        16: LiPO2F2 (additive only)
        17: NaClO4
        18: NaPF6
        19: NaBF4
        20: NaTFSI
        37: NaFSI
        21: PA5-PF6 (RTIL)
        22: PYR13-FSI (RTIL)
        23: EMIM-FSI or EMIM-FSI (RTIL)
        24: CsPF6
        25: Mg(TFSI)2

    For Aqueous Systems:
        17: NaClO4
        26: NaCl
        27: NaNO3
        28: Na2SO4
        29: LiNO3
        30: Li2SO4
        31: MgSO4
        32: Al(NO3)3
        33: LiBr
        34: NaOH
        35: KOH
        36: LiOH
        37: NaFSI

Note1: aqueous systems outside salts 25-31 have not been validated.
Note2: if an RTIL is chosen in a salt mixture, input the RTIL FIRST.

--> You have the option to designate a salt as an Arbitrarily-Chosen
Chemical Compound (ACCC), which may or may not be listed in the salt
library above. You may designate ONE ACCC salt per run, which can
be part of a two-salt mixture with a library salt.

ACCC salt parameters will be housed in and read from the file
    "ACCC Inputs (Salt Class)--suffix"
that you provide (input structure per K. Gering).

Do you wish to include one ACCC salt?

    0 for No,      1 for Yes

Input:
0

Choose non-ACCC salt(s) from library above:

Input number for salt 1 :
7
```

**Figure 134. Section A.5 from AEM Fortran Version 2.24.2.**

**A.8: Indicate maximum total salt concentration of interest:**

This is where the user defines the maximum concentration of salts. For battery electrolytes, this value falls between **6m to 8m**, where **m is molal units**. This value can reach upwards of **15m** when dealing with **aqueous systems**. As shown in Figure 135 for Example 1, we use **5m**.

```
A.8 Indicate maximum total salt concentration of interest.
(molal units, typically reaching 6 to 8m for battery electrolytes).
NOTE1: use care for conditions exceeding 5 molal total salt (non-aqueous).
NOTE2: can input up to 15 molal for some 1:1 salts (aqueous).
```

Value:

5

**Figure 135. Section A.8 from AEM Fortran Version 2.24.2.**

### 5.3.3 Section B: Input Other Simulation Conditions:

This section defines some other key parameters like the temperature profile, the method to handle Triple Ion Stability (ABA+ vs BAB-), and the inputs for electrolyte ingress into pores which are essential in simulating the user's desired electrolyte. This section contains 4 subsections described below.

#### B.1: Temperature Range.

This is where the user defines the temperature range in which the electrolyte will be used. There are two inputs for the temperature range, as follows.

- Minimum Temperature (**Input Tmin (C):**)
- Maximum Temperature (**Input Tmax (C):**)

The temperature range allowed by AEM will cover all conditions for electrolyte systems under conventional use conditions. A typical range for non-aqueous electrolytes is **-30°C to 60°C** with lower and higher temperatures possible. It is recommended not to exceed 100 °C. As shown in Figure 136, for Example 1, we use default inputs - **-30°C** for **Input Tmin (C)** and **60°C** for **Input Tmax (C)**.

```
B.1: Temperature Range. Calculation of properties over temperature
      is necessary to derive thermodynamic quantities.
      Specify minimum and maximum temperature of interest (degrees C),
      spanning at least 20 degrees.
      ==> Recommended typical range: -30 to 60 C. Do not exceed 100 C.
```

Note: Inputs will be adjusted to the nearest decade.

```
Input Tmin (C):
                  -30
Input Tmax (C):
                  60
```

**Figure 136. Section B.1 from AEM Fortran Version 2.24.2.**

**B.2: Input temperature stepsize for matrix and for outputs:**

This is where the user defines the step size for the temperature range that was specified in B.1. As shown in Figure 137, for Example 1, we use the **5°C** temperature step size.

```
B.2: Input temperature stepsize in matrix and for outputs:
    5 degrees C (finer grid; slightly better fidelity in Arrhenius calcs)
    10 degrees C (reduces matrix by nearly half; coarser Arrhenius calcs)

Value:
      5
```

**Figure 137. Section B.2 from AEM Fortran Version 2.24.2.**

**B.3: Input method for handling Triple Ion Stability (ABA+ vs BAB-):**

This is where the user chooses the preferred approach for triple ion stability, whether the default is used ( $[ABA+] = [BAB-]$ ) or whether there is subsequent conversion of either  $[ABA+]$  or  $[BAB-]$  into a single ion and an ion pair. As shown in Figure 138, for Example 1, we use **Option 1:  $[ABA+] = [BAB-]$  (default).** which will run

```
B.3: Input method for handling Triple Ion Stability (ABA+ vs BAB-):
  Option 1: [ABA+] = [BAB-] (default)
  Option 2: [ABA+] > [BAB-] due to BAB- --> B- + AB, or
            [ABA+] < [BAB-] due to ABA+ --> A+ + AB
            (these inequalities are automatically determined)

Input Option (1 or 2):
      1
```

**Figure 138. Section B.3 from AEM Fortran Version 2.24.2.**

**B.4: Inputs for Electrolyte Ingress into Pores:**

This is where the user defines three inputs correlating to the permeation of the electrolyte in porous regions, as follows. As shown in Figure 139, for Example 1 following are the inputs used.

- Contact Angle (**1. Contact Angle (0 to 90°)**) = **35°**
- Total Length of Pore (**2. Total Pore Length (0.1 to 50 micron)**) = **20μm**
- Concentration of Salt (**3. Salt Concentration of Interest (molal), must be less or equal to the maximum conc.)** = **1.5m**

```
B.4: Inputs for Electrolyte Ingress into Pores:  
    1. Contact Angle (0 to 90 degrees)  
    2. Total Pore Length (0.1 to 50 micron)  
    3. Salt Concentration of Interest (molal),  
       must be less or equal to the maximum conc.  
  
Input Contact Angle (value of 0 to 90):  
    35  
  
Input Total Pore Length (value of 0.1 to 50):  
    20  
  
Input Salt Concentration of Interest (value of 0.1 to 5.00000000 ):  
    1.5
```

**Figure 139. Section B.4 from AEM Fortran Version 2.24.2.**

#### **5.3.4 Section C: Choose whether Surface-Charge Attenuated Electrolyte Permittivity (SCAEP) Calculations are Performed:**

This section defines user inputs for calculation of surface-charge effects on permittivity for electrolyte neighboring an electrode surface. Local electrolyte permittivity will be reduced by the presence of an electrode surface charge as would be present during actual battery operation. As shown in Figure 140, for Example 1, we use **Input Choice: 0 for No** which will not run SCAEP calculations.

```
Section C: Choose whether Surface-Charge Attenuated Electrolyte Permittivity  
           (SCAEP) calculations are performed. These calculations will be  
           done at the solvent composition specified above and at conditions  
           chosen by the user. Other conditions are pre-set.  
           WARNING: SCAEP calculations take much CPU time and produce  
           large outputs  
  
Input Choice: 0 for No, 1 for Yes  
  
Input:  
    0
```

**Figure 140. Section C from AEM Fortran Version 2.24.2.**

### 5.3.5 Section D: Choose whether Double Layer (DL) Calculations are Performed:

This section defines user inputs to facilitate double-layer (DL) calculations. These calculations are done over a fine grid of spatial (1D, 5 nm steps) and time dimensions, allowing determination of electrolyte gradients and related properties in the anode and cathode double layers. These calculations are done over relatively short time periods to reveal the emergent dynamic of the electrolyte gradients. As shown in Figure 141, for Example 1, we use Input Choice: 0 for No which will not run DL calculations.

```
Section D: Choose whether Double Layer (DL) calculations are performed.  
DL calculations will be done at the starting composition of  
solvent proportions specified above and a chosen salt concentration.  
Basis: constant-current conditions over pulse time (pre-set).  
Default cell voltage of 4.0V is assigned.  
WARNING: DL calculations take much CPU time, produce large outputs,  
and not every choice of conditions will converge.  
  
Input Choice: 0 for No, 1 for Yes  
  
Input:  
0
```

Figure 141. Section D from AEM Fortran Version 2.24.2.

### 5.3.6 Section E: Output Files

When all the simulations settings are supplied, AEM starts the simulation run. AEM then updates the data output report files with the simulation results. As shown in **Figure 142**, the AEM CLI will prompt the user to run another set of conditions (**1 = Yes**) which will append the data output files or exit the program (**0 = No**).

Note that if the software is restarted, then previously generated data output files will be overwritten. These files should be copied to another folder for future use if desired or use the GUI which organizes them in a timestamped directory.

```
Depending on input choices, AEM is generating Reports covering Key Topics:
```

```
Report1 -- Highlighted Quantities
Report2 -- Ionic Speciation, Thermodynamic and Equilibrium Quantities
Report3 -- GFE and Ion Solvation Energies; Permittivity Terms
Report4 -- Diffusivities and selected conductivity terms
Report5 -- Transport Properties (viscosity, conductivity, etc.)
Report6 -- Arrhenius Analyses for Key Quantities
Report7 -- Optimization Results (multi-solvent matrix)
Report8 -- Non-convergent cases
Report9 -- Double Layer (DL) Analyses (if chosen; extensive CPU time)
Report10 -- Surface Charge Effects on Electrolyte Permittivity
Report11 -- Comprehensive Ion Solvation Quantities
Report12 -- Preferential Ion Solvation Quantities
Report13 -- Factors that Impact Ionic Conductivity (cation and anion)
Report14 -- Li-STEP terms
Report15 -- Cation and solvent velocities and transit times per dV/dx
Report16 -- Surface Tension and pore filling time over salt conc.
Report17 -- Percent pore length filled over time
Report18 -- Ligand-wise cation desolvation energy and time
Report19 -- Ligand-wise cation desolvation energy and time (accounting for CS)
Report20 -- Terms relating to structure and Communal Ion Solvation (CS)
```

```
All inputs received. Calculations have started.....
```

```
.....Calculations have finished.
```

```
Do you wish to perform another set of conditions?
```

```
0 = No
1 = Yes
```

```
(additional results will be added at the end of current output files)
```

```
Input 0 or 1
```

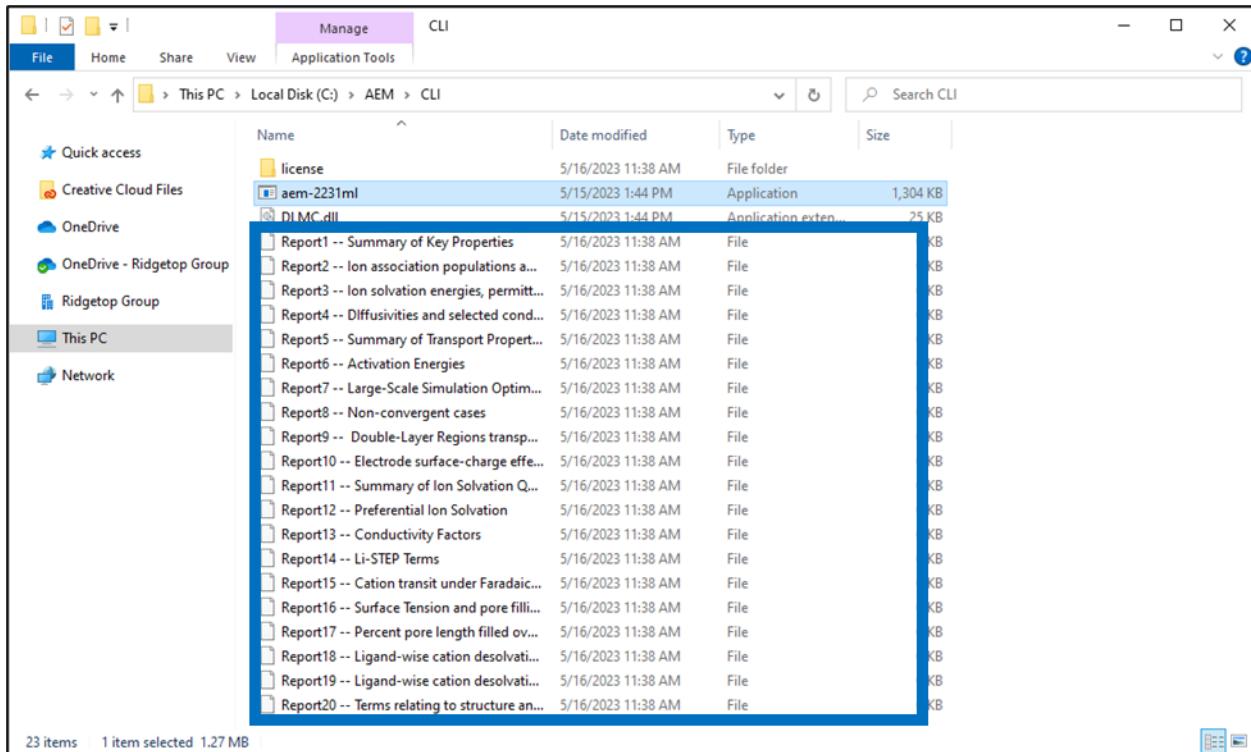
```
0
```

**Figure 142. Section E from AEM Fortran Version 2.24.2.**

The final output reports can be found in ...\\AEM\\CLI\\ as shown in Figure 143.

Congratulations! You have successfully run Example 1 using the AEM CLI if you make it to this stage without any errors.

## Advanced Electrolyte Model (AEM)

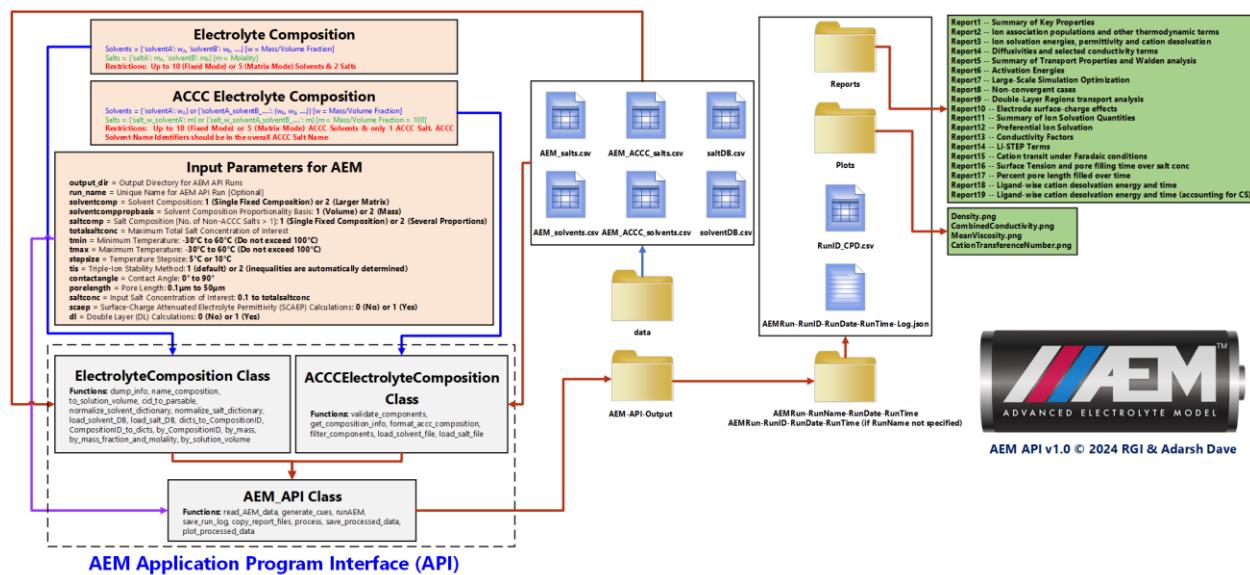


**Figure 143. The different output files generated by AEM are highlighted inside the blue box.**

## 6 AEM Python API

The Advanced Electrolyte Model (AEM) Application Program Interface (API) is a supporting software toolbox to the AEM CLI executable, designed to analyze and predict the properties of electrolyte compositions used in various applications. Developed by Ridgetop Group, Inc. and in collaboration with Adarsh Dave (Carnegie Mellon University), this API allows users to create, manage, and simulate electrolyte compositions with Python scripts, leveraging the extensive databases of non-ACCC as well as ACCC solvents and salts with the AEM compound library. Additionally, the API combines results from AEM output Report 1, saves that to a .csv file, and provides detailed insights into example key properties such as density, viscosity, conductivity, and ion association populations through graphical plots.

### 6.1 API Architecture



**Figure 144. The modular AEM API Architecture.**

Shown in Figure 144 is a block diagram of the AEM API v1.0 architecture. The diagram is divided into several sections, each elaborating on different aspects of the AEM API, from input parameters to outputs, classes, and reports.

On the **user level**, there are three major inputs - **Electrolyte Composition**, **ACCC Electrolyte Composition**, and **Input Parameters**. In the Electrolyte Composition, the user can define up to 10 solvents (fixed mode) or 5 solvents (matrix mode) and up to two salts. In the ACCC Electrolyte Composition, the user can define up to 10 ACCC solvents (fixed mode) or 5 ACCC solvents (matrix mode) and only one ACCC salt. The ACCC salt chosen must contain all the identifiers for the chosen ACCC solvent. The user can choose between a pure non-ACCC composition, a pure ACCC composition, or a cross composition between non-ACCC and ACCC components. Next, Input Parameters lists the various inputs required for running AEM CLI executable. These inputs are

essential for configuring AEM simulation runs and determining the specific conditions under which the model operates.

Within the **API itself (AEM\_API.py)** there are three classes - the **ElectrolyteComposition Class**, the **ACCCElectrolyteComposition Class**, and the **AEM\_API Class**. The ElectrolyteComposition Class includes functions for managing the non-ACCC composition, whereas the ACCCElectrolyteComposition Class includes functions for managing the ACCC composition. The AEM\_API Class contains functions for reading inputs, generating compositions, running simulations using the AEM CLI program, saving logs, exporting files and results, processing data, and saving processed data.

The **Outputs** from the API are organized into the **AEM\_API\_Output** directory in run directories with the name **AEMRun-RunID-RunDate-RunTime**. Each run directory includes the **Reports** and **Plots** folders along with the combined processed data .csv file (**RunID-CPD.csv**) and a run log .json file (**AEMRun-RunID-RunDate-RunTime-Log.json**). The Reports folder contains different types of reports that the AEM CLI program can generate. These reports cover a wide range of analyses, from key properties summaries and thermodynamic terms to density, viscosity, conductivity, and cation desolvation. Other reports focus on dielectric analysis, transport properties, molar volume, ion-pair formation, self-diffusion coefficients, and ligand-wise analyses, among others. Each report provides detailed insights into specific aspects of the electrolyte compositions and their behaviors under various conditions. The Plots folder contains visual plots for various electrolyte properties.

## 6.2 Requirements and Dependencies

This section outlines the necessary requirements and dependencies required to run the Advanced Electrolyte Model (AEM) API. Ensuring these dependencies are installed correctly is essential for running the AEM API as defined in this User Guide.

- **Visual Studio Code:** Visual Studio Code Version 1.92 or higher ([Download Visual Studio Code - Mac, Linux, Windows](#))
- **Python:** Python 3.7 or higher ([Download Python | Python.org](#))
- **Git:** 2.46.0 or higher ([Git - Downloading Package \(git-scm.com\)](#))

Below is a list of the Python libraries and dependencies required to run the AEM API. Each library serves a specific purpose in the workflow.

1. **subprocess:** This module allows you to spawn new processes, connect to their input/output/error pipes, and obtain their return codes. It is used for running external commands and programs from within the script. is part of the standard Python library, so no separate installation is required.
2. **pandas:** A powerful data manipulation and analysis library. It is used for handling and processing data structures like DataFrames. Can be installed by running - `pip install pandas`

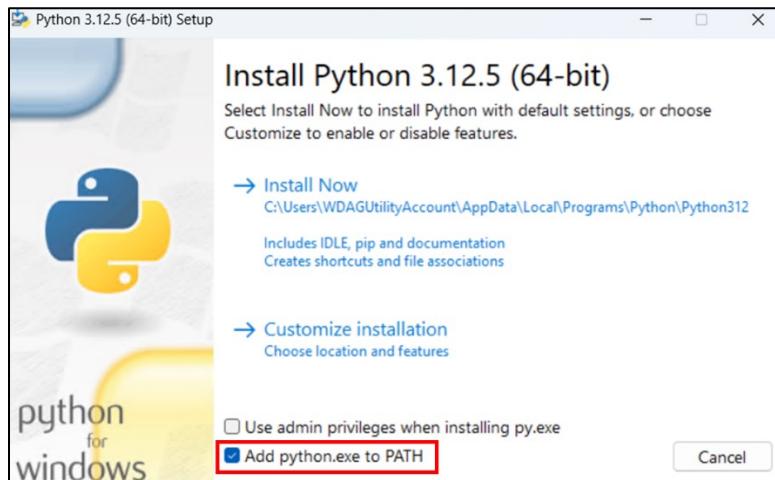
3. **matplotlib**: A plotting library used for creating static, animated, and interactive visualizations in Python. Can be installed by running - `pip install matplotlib`
4. **re**: The re module provides regular expression matching operations. It is part of the standard Python library, so no separate installation is required.
5. **collections**: The collections module implements specialized container datatypes like OrderedDict. It is part of the standard Python library.
6. **OrderedDict**: This class is a dictionary that remembers the order in which its contents are added.
7. **datetime**: This module supplies classes for manipulating dates and times. It is part of the standard Python library.
8. **json**: This module provides an easy way to encode and decode data in JSON format. It is part of the standard Python library.
9. **uuid**: This module provides immutable UUID objects (universally unique identifiers) and the functions to generate them. It is part of the standard Python library.
10. **os**: This module provides a way of using operating system-dependent functionality like reading or writing to the file system. It is part of the standard Python library.
11. **sys**: This module provides access to some variables used or maintained by the Python interpreter and to functions that interact strongly with the interpreter. It is part of the standard Python library.
12. **shutil**: This module offers a number of high-level operations on files and collections of files. It is part of the standard Python library.

## 6.3 Installation and Execution

### Step 1: Preparation

These are some initial steps to be followed before cloning the AEM API repository from GitHub to your local machine.

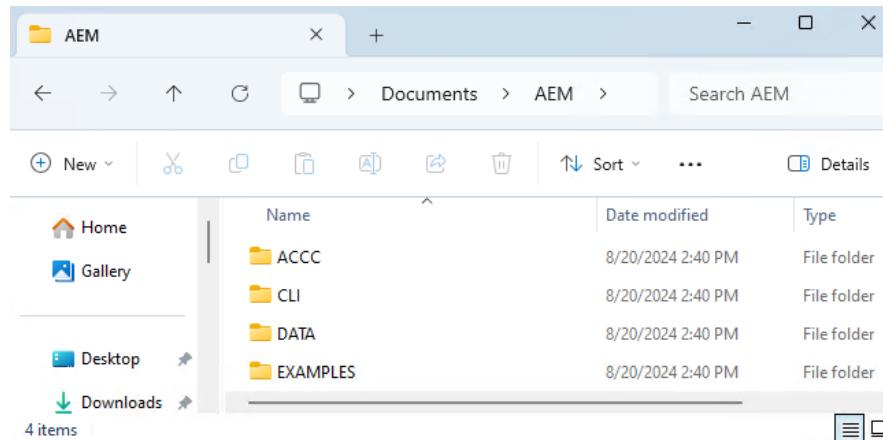
1. Download and install each main dependency defined in Section 6.2 for Visual Studio Code, Python, and Git. Note that the “Add python.exe to PATH” checkbox should be selected as shown in Figure 145.



**Figure 145. Selecting the option python.exe checkbox during the Python installation.**

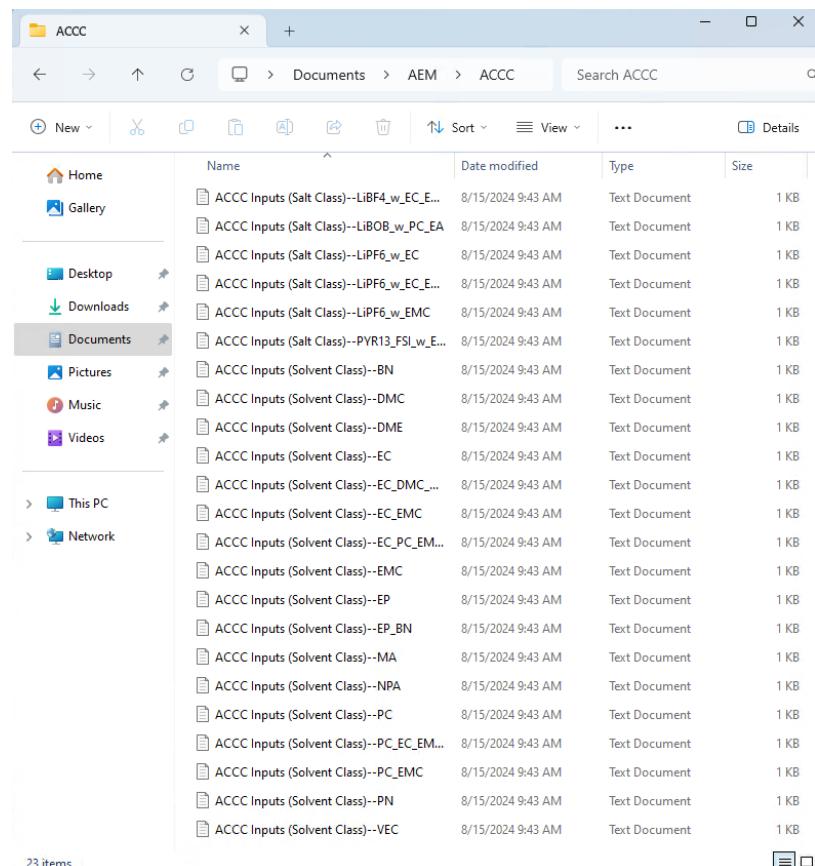
## Advanced Electrolyte Model (AEM)

2. Install AEM as described in Section 2.
3. Make sure default AEM directory is set to **C:\Users\user-name\Documents\AEM\** and the directories shown below exist within it as shown in Figure 146.



**Figure 146. The folder structure for the default AEM directory.**

4. Copy all/required ACCC compositions as shown in Figure 147, within the **ACCC\** directory, to the **CLI\** directory.



**Figure 147. ACCC compositions within the ACCC\ directory.**

5. Note that default AEM directory is organized with the following subdirectories:

<b>C:\Users\user-name\Documents\AEM\</b>	<b>Executable subdirectory</b>
1. ACCC\	AEM ACCC Composition Files
2. CLI\	AEM Command Line Interface Directory
3. DATA\	AEM Data Output Files
4. EXAMPLES\	AEM Example Files

## Step 2: Open Visual Studio Code and Clone the Repository from GitHub

1. Next, open Visual Studio Code, select File>Open Folder, and open the default AEM directory as shown in Figure 148. Note, that the Windows PowerShell / Terminal can be added to the bottom of the VS Code window by selecting View>Terminal.

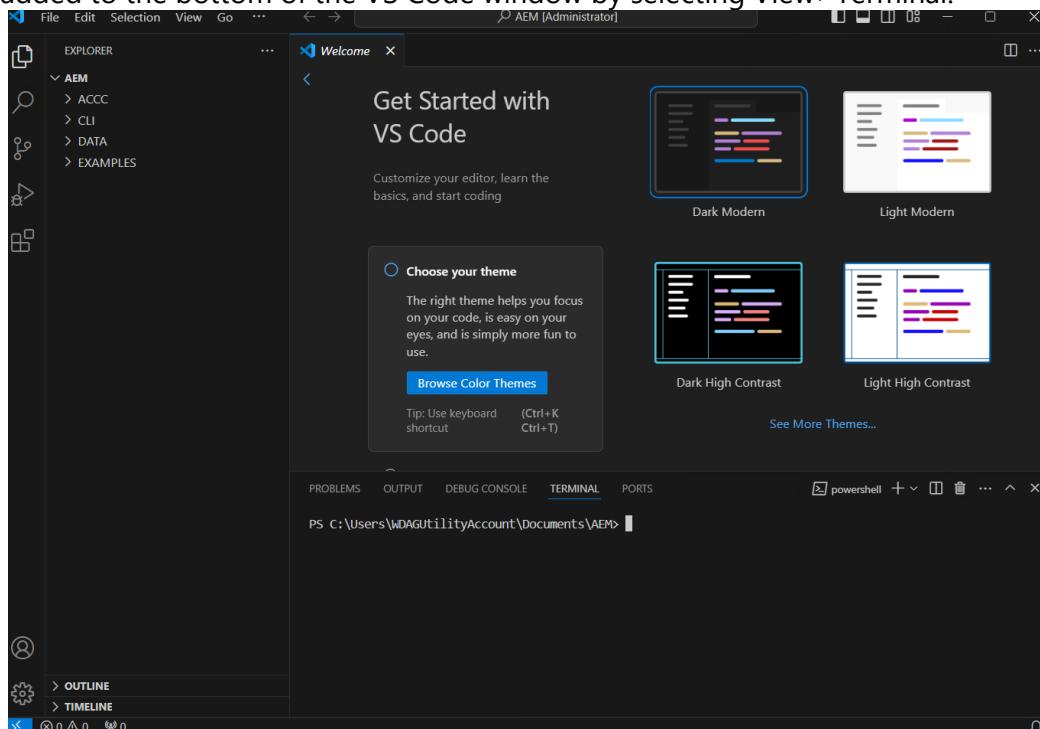


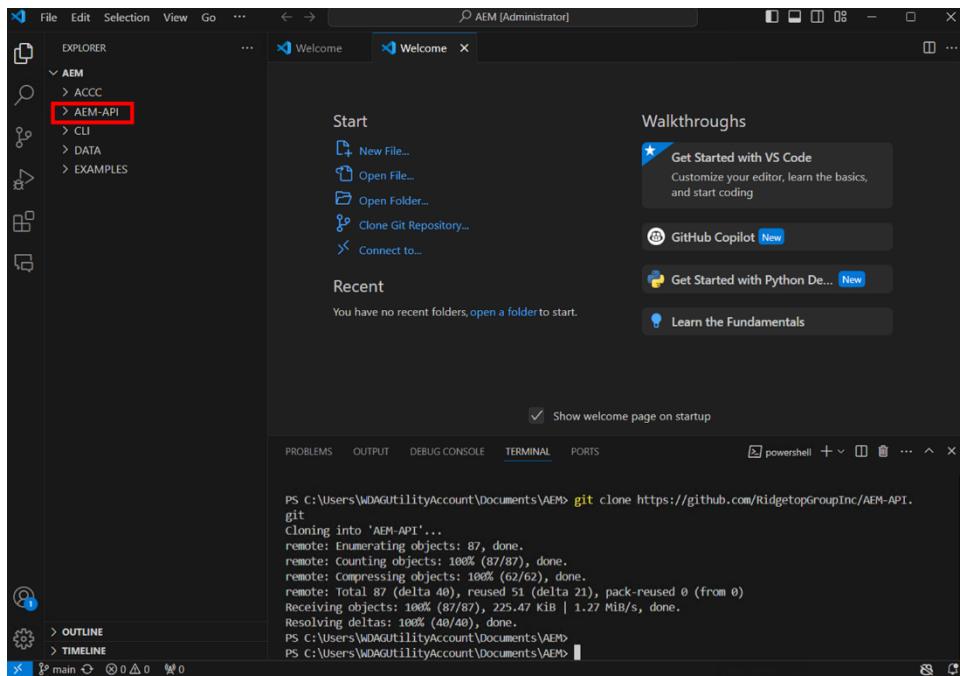
Figure 148. Opening default AEM user directory in VS Code.

2. Run the following command to clone from Github:

```
git clone https://github.com/RidgetopGroupInc/AEM-API.git
```

3. Verify this command created a directory named **AEM-API** in the **AEM\** directory with all the files from the repository as shown in Figure 149.

## Advanced Electrolyte Model (AEM)



**Figure 149. View of VS Code Window after cloning AEM-API from Github.**

4. Using the Terminal in VS Code, navigate to the **AEM-API** repository directory and install the required dependencies using the following commands.

```
cd AEM-API  
pip install -r requirements.txt
```

Note: If you encounter any errors, verify that the "Add Python to environment variables" checkbox was selected during the Python installation and confirm that the **requirements.txt** file is located in the root directory of the cloned repository, listing all required dependencies.

5. Verify that the Terminal in VS Code shows a successful installation for all dependencies in the **requirements.txt** file as shown in Figure 150.

```
PS C:\Users\WDAGUtilityAccount\Documents\AEM\AEM-API> pip install -r requirements.txt
Requirement already satisfied: numpy in c:\users\wdagutilityaccount\appdata\local\programs\python\python312\lib\site-packages (from -r requirements.txt (line 1)) (2.1.0)
Collecting pandas (from -r requirements.txt (line 2))
  Downloading pandas-2.2.2-cp312-cp312-win_amd64.whl.metadata (19 kB)
Collecting matplotlib (from -r requirements.txt (line 3))
  Downloading matplotlib-3.9.2-cp312-cp312-win_amd64.whl.metadata (11 kB)
Collecting python-dateutil>=2.8.2 (from pandas->r requirements.txt (line 2))
  Downloading python_dateutil-2.9.0.post0-py2.py3-none-any.whl.metadata (8.4 kB)
Collecting pytz>=2020.1 (from pandas->r requirements.txt (line 2))
  Downloading pytz-2024.1-py2.py3-none-any.whl.metadata (22 kB)
Collecting tzdata>=2022.7 (from pandas->r requirements.txt (line 2))
  Downloading tzdata-2024.1-py2.py3-none-any.whl.metadata (1.4 kB)
Collecting contourpy>=1.0.1 (from matplotlib->r requirements.txt (line 3))
  Downloading contourpy-1.2.1-cp312-cp312-win_amd64.whl.metadata (5.8 kB)
Collecting cycler>=0.10. (from matplotlib->r requirements.txt (line 3))
  Downloading cycler-0.12.1-py3-none-any.whl.metadata (3.8 kB)
Collecting fonttools>=4.22.0 (from matplotlib->r requirements.txt (line 3))
  Downloading fonttools-4.53.1-cp312-cp312-win_amd64.whl.metadata (165 kB)
Collecting kiwisolver>=1.3.1 (from matplotlib->r requirements.txt (line 3))
  Downloading kiwisolver-1.4.5-cp312-cp312-win_amd64.whl.metadata (6.5 kB)
Collecting packaging>=20.0 (from matplotlib->r requirements.txt (line 3))
  Downloading packaging-24.1-py3-none-any.whl.metadata (3.2 kB)
Collecting pillow>=8 (from matplotlib->r requirements.txt (line 3))
  Downloading pillow-10.4.0-cp312-cp312-win_amd64.whl.metadata (9.3 kB)
Collecting pyparsing>=2.3.1 (from matplotlib->r requirements.txt (line 3))
  Downloading pyparsing-3.1.2-py3-none-any.whl.metadata (5.1 kB)
Collecting six>=1.5 (from python-dateutil>=2.8.2->pandas->r requirements.txt (line 2))
  Downloading six-1.16.0-py2.py3-none-any.whl.metadata (1.8 kB)
Downloading pandas-2.2.2-cp312-cp312-win_amd64.whl (11.5 MB)
  11.5/11.5 MB 32.7 MB/s eta 0:00:00
Downloading matplotlib-3.9.2-cp312-cp312-win_amd64.whl (7.8 MB)
  7.8/7.8 MB 48.5 MB/s eta 0:00:00
Downloading contourpy-1.2.1-cp312-cp312-win_amd64.whl (189 kB)
Downloading cycler-0.12.1-py3-none-any.whl (8.3 kB)
Downloading fonttools-4.53.1-cp312-cp312-win_amd64.whl (2.2 MB)
  2.2/2.2 MB 20.5 MB/s eta 0:00:00
Downloading kiwisolver-1.4.5-cp312-cp312-win_amd64.whl (56 kB)
Downloading packaging-24.1-py3-none-any.whl (53 kB)
Downloading pillow-10.4.0-cp312-cp312-win_amd64.whl (2.6 MB)
  2.6/2.6 MB 49.8 MB/s eta 0:00:00
Downloading pyparsing-3.1.2-py3-none-any.whl (103 kB)
Downloading python_dateutil-2.9.0.post0-py2.py3-none-any.whl (229 kB)
Downloading pytz-2024.1-py2.py3-none-any.whl (505 kB)
Downloading tzdata-2024.1-py2.py3-none-any.whl (345 kB)
Downloading six-1.16.0-py2.py3-none-any.whl (11 kB)
Installing collected packages: pytz, tzdata, six, pyparsing, pillow, packaging, kiwisolver, fonttools, cycler, contourpy, python-dateutil, pandas, matplotlib
Successfully installed contourpy-1.2.1 cycler-0.12.1 fonttools-4.53.1 kiwisolver-1.4.5 matplotlib-3.9.2 packaging-24.1 pandas-2.2.2 pillow-10.4.0 pyparsing-3.1.2 python-dateutil-2.9.0.post0 pytz-2024.1 six-1.16.0 tzdata-2024.1
```

**Figure 150.** A visual of the command line while installing dependencies.

### Step 3: Running the AEM API Scripts

The following Python scripts are provided to simulate different AEM scenarios.

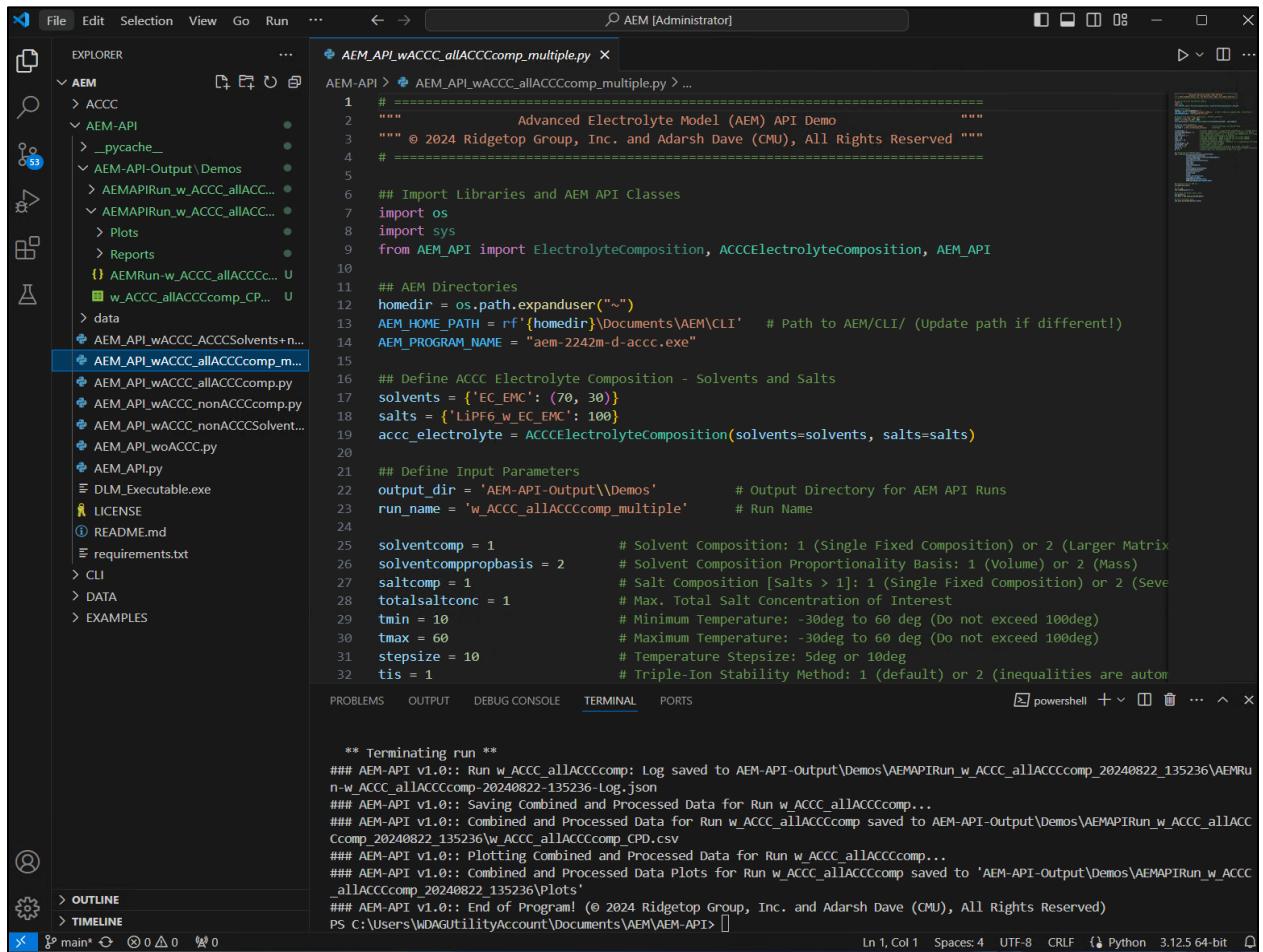
1. **AEM\_API\_woACCC.py** – No ACCC Functionality, with pure non-ACCC composition
2. **AEM\_API\_wACCC\_nonACCCcomp.py** – ACCC, with pure non-ACCC composition
3. **AEM\_API\_wACCC\_allACCCcomp.py** – ACCC, with pure ACCC composition
4. **AEM\_API\_wACCC\_allACCCcomp\_multiple.py** – ACCC, with pure ACCC composition (multiple solvents)
5. **AEM\_API\_wACCC\_ACCTSolvents+nonACCCSalt.py** – ACCC, 2 ACCC Solvents + 1 Non-ACCC Salt
6. **AEM\_API\_wACCC\_nonACCCSolvents+ACCCSalt.py** – ACCC, 2 Non-ACCC Solvents + 1 ACCC Salt

They can be run by passing the following command from within the **AEM-API\** directory.

```
python AEM_API_ScriptName.py
```

An example is shown in Figure 151, where the **AEM\_API\_wACCC\_allACCCcomp.py** is run from the Terminal in VS Code.

## Advanced Electrolyte Model (AEM)



The screenshot shows the Visual Studio Code interface with the following details:

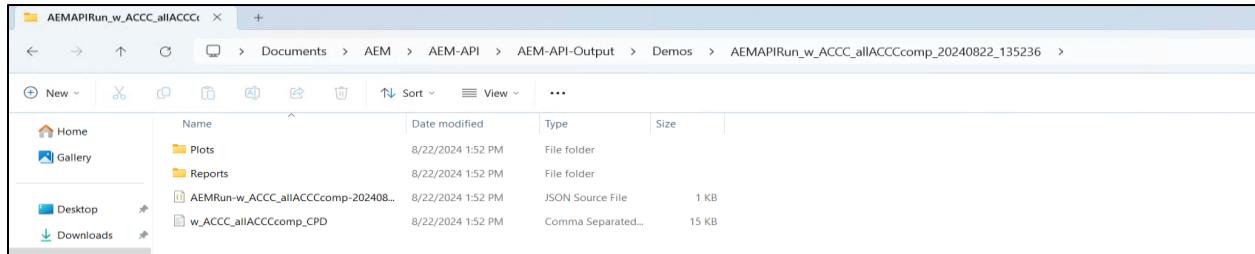
- File Explorer:** Shows the project structure under the 'AEM' folder, including subfolders like 'ACCC', 'AEM-API', '\_pycache\_\_', 'AEM-API-Output\Demos', 'Plots', 'Reports', and various Python files.
- Code Editor:** Displays the content of the file 'AEM\_API\_wACCC\_allACCCcomp\_multiple.py'. The code defines parameters for a multi-component electrolyte simulation, including solvent and salt types, their proportions, and temperature ranges. It also specifies the output directory and run name.
- Terminal:** Shows the command-line output of the script execution. It includes messages about terminating the run, saving logs, and combined processed data to a timestamped directory ('AEMAPIRun\_w\_AC...').
- Status Bar:** Provides information about the current session, such as the file type (Python), version (3.12.5), and bit width (64-bit).

**Figure 151.** A visual from VS Code when the when `AEM_API_wACCC_allACCCcomp.py` script is run from the Terminal.

The output results can be viewed by opening a File Explorer and navigating to the following directory:

- C:\Users\user-name\Documents\AEM\AEM-API\AEM-API-Output\Demos\

Note that the AEM-API saves the output reports and automatically processed data plots in a time stamped directory as shown in Figure 152:



**Figure 152.** View of data output directory from AEM simulation using Python API.

## 6.4 AEM API Usage

### 6.4.1 AEM Home Path and Program Name Setup

To begin with, ensure that the AEM home path and program name are correctly set up in your Python script.

Example configuration in your Python script:

```
## AEM Directories
homedir = os.path.expanduser("~")
AEM_HOME_PATH = rf'{homedir}\Documents\AEM\CLI'
AEM_PROGRAM_NAME = "aem-2242m-d-accc.exe"
```

Replace **AEM\_HOME\_PATH** to the correct path where the AEM executable is located if it is not set to **default** (`C:\Users\<username>\Documents\AEM\CLI`).

**Important Note:** The current AEM Program Name is **aem-2242m-d-accc.exe** which corresponds to v2.1.9. The API is backward compatible for any version of AEM higher than v2.1.0. Get in touch with Ridgetop should you need a backward compatible version of the API.

### 6.4.2 Define Electrolyte Compositions

The first step is to define the composition of the solvents and salts you will use in your electrolyte model. The user can define either a non-ACCC or ACCC compositions, or both.

#### Non-ACCC Electrolyte Composition

In this example we define the solvents EMC and EC with mass fractions of 0.7 and 0.3, respectively, and the salt LiPF6 with a molality of 1.

```
## Define Electrolyte Composition - Solvents and Salts
solvents = {'EMC': 0.7, 'EC': 0.3}
salts = {'LiPF6': 1}
electrolyte_comp = ElectrolyteComposition.by_mass_fraction_and_molality(solvents=solvents, salts=salts)
```

#### ACCC Electrolyte Composition

**Important Note:** Only 1 ACCC Salt can be used with any given number of ACCC solvents.

In this example we define the ACCC solvent EC with mass percentage of 100% and the ACCC salt LiPF6 with a mass percentage of 100% as well.

```
## Define ACCC Electrolyte Composition - Solvents and Salts
solvents = {'EC': (100)}
salts = {'LiPF6_w_EC': 100}
accc_electrolyte = ACCCElectrolyteComposition(solvents=solvents, salts=salts)
```

In the example below, a case with multiple ACCC solvents is shown where we define the ACCC solvent EC\_EMCC, consisting of EC and EMC, with mass percentages of 70% and 30%, respectively, and the ACCC salt LiPF6\_w\_EC\_EMCC with a mass percentage of 100%.

**Important Note:** If multiple ACCC solvents are being used, the ACCC solvent names ( $S_1.S_2..S_n$ ) should match the ACCC salt name (Salt\_w\_ $S_1.S_2..S_n$ ).

```
## Define ACCC Electrolyte Composition - Solvents and Salts
solvents = {'EC_EMCC': (70, 30)}
salts = {'LiPF6_w_EC_EMCC': 100}
accc_electrolyte = ACCCElectrolyteComposition(solvents=solvents, salts=salts)
```

### 6.4.3 Define Input Parameters

Next, set the necessary parameters for the AEM API. These parameters control the conditions and settings for your model and are essential for defining the conditions under which the electrolyte properties will be evaluated.

```
## Define Input Parameters
output_dir = 'AEM-API-Output\\Demos' # Output Directory for AEM API Runs
run_name = 'w_ACAC_allACCCcomp' # Run Name
```

```
solventcomp = 1 # Solvent Composition: 1 (Single Fixed Composition) or 2 (Larger Matrix)
solventcomppropbasis = 2 # Solvent Composition Proportionality Basis: 1 (Volume) or 2 (Mass)
saltcomp = 1 # Salt Composition [Salts > 1]: 1 (Single Fixed Composition) or 2 (Several Proportions)
totalsaltconc = 1 # Max. Total Salt Concentration of Interest
tmin = 10 # Minimum Temperature: -30deg to 60 deg (Do not exceed 100deg)
tmax = 60 # Maximum Temperature: -30deg to 60 deg (Do not exceed 100deg)
stepsize = 10 # Temperature Stepsize: 5deg or 10deg
tis = 1 # Triple-Ion Stability Method: 1 (default) or 2 (inequalities are automatically determined)
contactangle = 90 # Contact Angle: 0deg to 90deg
porelength = 50 # Pore Length: 0.1um to 50um
saltconc = 0.1 # Input Salt Concentration of Interest: 0.1 to Max. Salt Conc.
scaepl = 0 # Surface-Charge Attenuated Electrolyte Permittivity (SCAEPL) Calculations: 0 (No) or 1 (Yes)
dl = 0 # Double Layer (DL) Calculations: 0 (No) or 1 (Yes)
```

### 6.4.4 Initialize and Run the AEM API

Initialize the AEM API object with the defined electrolyte composition and input parameters, and then run the model. Here, we initialize the **AEM\_API** object with the electrolyte composition and input parameters, then the **generate\_cues()** method prepares the necessary cues for running the AEM CLI, and the **runAEM()** method executes the AEM model. The **quiet=True** parameter suppresses verbose output.

```

## Initialize the AEM-API Object
aem = AEM_API(accc_electrolyte=accc_electrolyte,
               solventcomp=solventcomp,
               solventcomppropbasis=solventcomppropbasis,
               saltcomp=saltcomp,
               totalsaltconc=totalsaltconc,
               tmin=tmin,
               tmax=tmax,
               stepsize=stepsize,
               tis=tis,
               contactangle=contactangle,
               porelength=porelength,
               saltconc=saltconc,
               scaep=scaep,
               dl=dl,
               output_dir=output_dir,
               run_name=run_name,
               AEMHomePath=AEM_HOME_PATH,
               AEMProgramName=AEM_PROGRAM_NAME)

## Generate Cues for AEM CLI
aem.generate_cues()

## Run AEM
aem.runAEM(quiet=False)

```

## Process and Plot the Output Data

After running the AEM model, the next steps are to process the output data and create visualizations. Here, the **aem.process()** method processes the raw output data generated by the AEM model. It typically involves cleaning, transforming, and organizing the data into a structured format. The **aem.save\_processed\_data()** method saves the processed data to a specified location. The **all\_data** variable will contain the processed data, which can be used for further analysis or plotting. Finally, the **aem.plot\_processed\_data(all\_data)** method takes the processed data (**all\_data**) as input and generates plots.

```

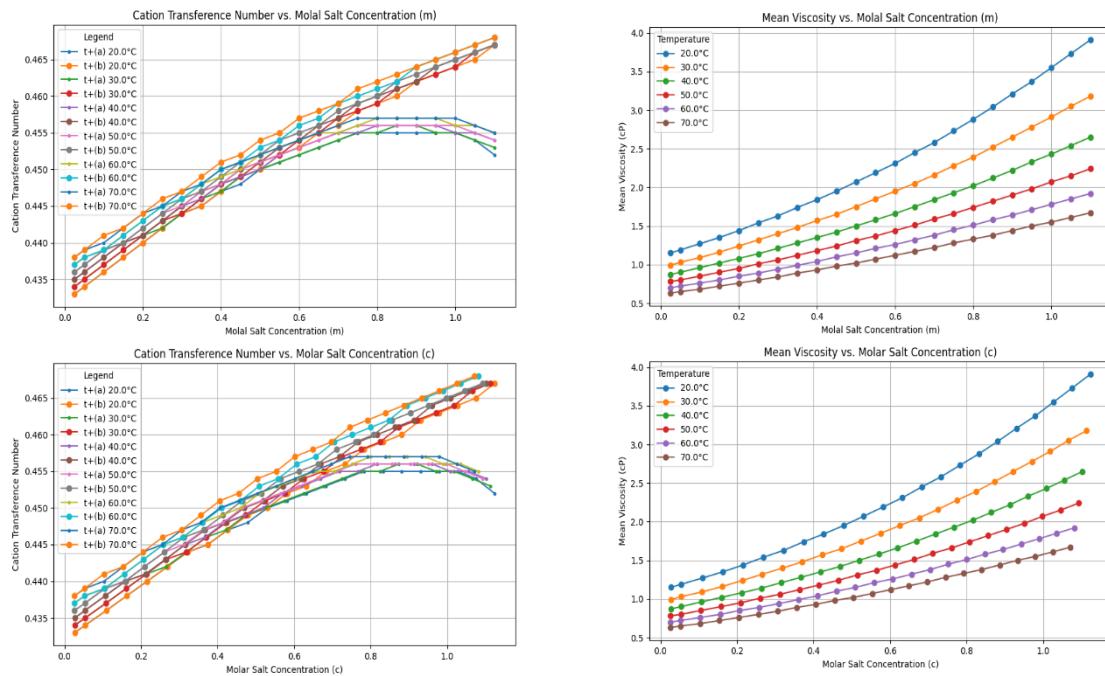
## Process the Output Data & Save
aem.process()
all_data = aem.save_processed_data()

## Plot the Output Data
aem.plot_processed_data(all_data)

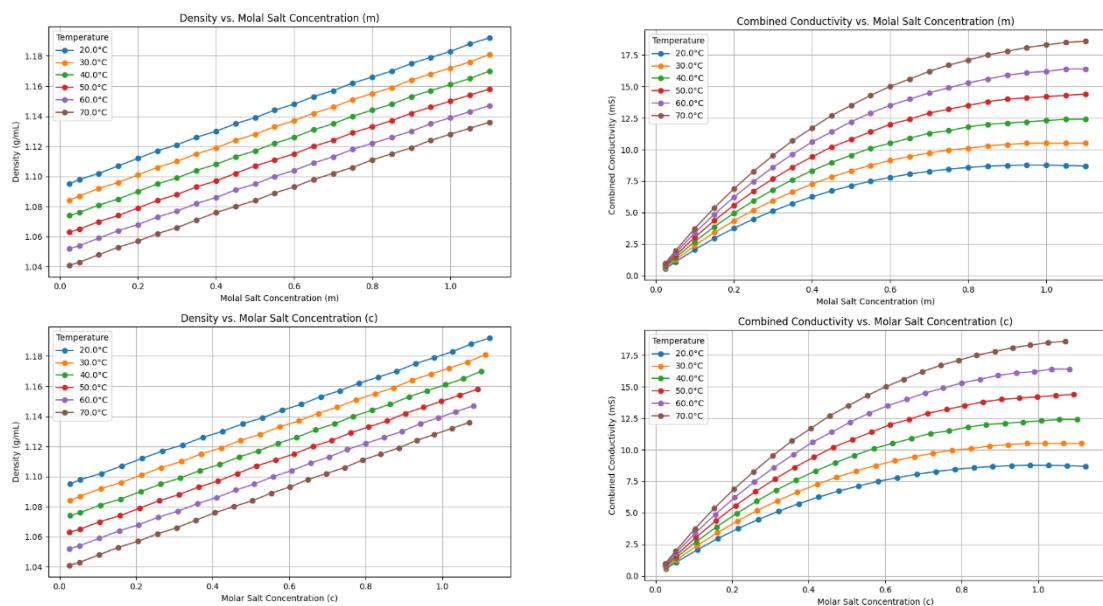
```

Following are the plots generated by the program.

## Advanced Electrolyte Model (AEM)



**Figure 153. Cation Transference No. [t+(a) & t+(b)] (left) and Mean Viscosity (right) as a function of Molal (m) and Molar (c) Salt Concentrations.**



**Figure 154. Density (g/mL) (left) and Combined Conductivity (right) as a function of Molal (m) and Molar (c) Salt Concentrations.**

## 7 Appendix

### 7.1 AEM Data Output Summary

#### 7.1.1 Summary Table of AEM Outputs

Quantity	Definition/Description	Importance and Application Areas
<b>Solvated Ion Sizes (cation, anion)</b> - Hard sphere basis - Effective transport basis	Chemical Physics property directly relevant to extent of ion solvation over conditions of state (temperature, salt conc., solvent composition)	Ionic transport and conductivity in electrochemical systems; metal ion transport in metabolic processes. Also influences thermodynamic metrics such as activity coefficients
<b>Solvent-to-ion Binding Energies (cation, anion)</b>	Thermodynamic property directly relevant to extent of ion solvation over conditions of state (temperature, salt conc., solvent composition)	Ion desolvation energy requirements in charge transfer process in electrochemical systems, and in metabolic processes
<b>Solvation Numbers (cation, anion, ion-associated species)</b>	Thermodynamic property that represents the number of solvent species that reside in close proximity to ions.	Impacts kinetics and energetics of ion desolvation processes in electrochemical systems, as well as solvent co-transport in a number of electrolyte-centric processes.
<b>Ion Desolvation Energy</b>	Net energy involved in solvent-wise ion desolvation based on the solvation number at a given condition (cation).	Quantifies the energy required to overcome lithium solvation prior to lithium (or other) ion charge transfer and insertion into host. Analogs exist in terms of metabolic processes.
<b>Ion Desolvation Kinetics</b>	Net time required for solvent-wise ion desolvation based on the solvation number at a given condition (cation).	Quantifies the time required to overcome lithium solvation prior to lithium (or other) ion charge transfer and insertion into host. Analogs exist in terms of metabolic processes.

Quantity	Definition/Description	Importance and Application Areas
<b>Comprehensive evaluation of species populations: cation, anion, ion pairs, triple ions, solid solvates</b>	Correct equilibrium speciation of all components by thermodynamic Mass Action Law analyses	Impacts macro-scale properties that are dependent on the extent of free ions (conductivity, diffusivity) and net solvation behavior (viscosity). This is a crucial metric within electrochemical double layers.
<b>Solution Permittivity Solvent Permittivity</b>	Represents true dielectric of solvent and solution according to “dielectric depression” that occurs due to the presence of ionic fields. Calculated over conditions of state (temperature, salt conc., solvent composition)	Dielectric depression will influence the extent of ion association, which in turn impacts properties like conductivity and diffusivity.
<b>Relative molal enthalpy</b>	Thermophysical property tied to heat capacity, calculated over conditions of state (temperature, salt conc., solvent composition)	Important to thermal issues involving electrolyte, such as heat transfer.
<b>Density</b>	Mass electrolyte per unit volume	Related to partial molar volume of electrolyte.
<b>Mean activity coefficient of salt</b> - Rational basis - Practical basis	Describes the extent of non-ideality introduced by presence of solvated charged species	Crucial thermodynamic metric for issues pertaining to electrolyte equilibrium per state conditions
<b>Osmotic coefficient (and Osmotic Pressure)</b>	Characterizes how the presence of a dissolved solute causes deviation of a solvent from ideal behavior, using a reference state such as pure solvent	Crucial thermodynamic metric for issues pertaining to the equilibrium state per state conditions; related to solvent activity

Quantity	Definition/Description	Importance and Application Areas
<b>Viscosity</b>	Physical property that characterizes a fluid's resistance to flow	Key transport property inversely related to conductivity and diffusivity. Viscosity is most problematic at low temperatures and high salt concentrations.
<b>Conductivity (ion-wise, net)</b>	Electronic property that characterizes the ability to pass current, here through ionic mobility; inverse to resistivity.	The premier transport property in terms of battery electrolytes. Used extensively in transport analysis. One of the most-oft measured and published properties of electrolytes of electrochemical systems.
<b>Diffusivity (ion-wise; solvent)</b>	Physical property tied to the diffusive propensity (Fickian) of labile species.	Also used in chemical and electrochemical transport calculations. Important where concentration gradients emerge (double layers) due to battery cycling conditions.
<b>Transference Numbers</b>	Electrochemical property that represents the fraction of the total electric current that cations and anions carry in passing through an electrolytic solution. The cationic term is usually of interest.	High cationic transference numbers indicate that a battery electrolyte is more suited for higher-power applications.
<b>Ion Hopping</b> - cation - anion	The statistical fraction of path length wherein an ion is minimally solvated under Faradaic transport.	Ion hopping is one of the most efficient modes of transport in electrolyte systems. The goal is to find electrolytes and conditions therein that promote ion hopping.

Quantity	Definition/Description	Importance and Application Areas
<b>Communal Solvation (CS)</b>	The fraction of solvent in an electrolyte that is involved in multi-ion solvation or simultaneous solvation per solvent molecule.	CS contributes to higher electrolyte viscosity because it introduces structure on the molecular scale, and it can complicate the ion desolvation process. In some applications (batteries) low values of CS are sought, while in other applications (solvent-based extraction) high values are desirable.
<b>Li-STEP</b>	Lithium ion Solvation and Transport Electrolyte Parameter is a term that incorporates salient macro-scale transport terms with molecular scale desolvation energy and kinetics.	Serves as a convenient overall screening metric for evaluating electrolyte systems for batteries.
<b>Electrolyte properties in double layer (DL) under conditions of non-electroneutrality</b>	While performing transport calculations AEM calculates the dynamic change of electrolyte conc. and properties within DL regions as concentration polarization causes speciation over pulse time.	Non-electroneutrality can occur in a double layer, and the electrolyte properties of such a resultant region are nearly impossible to predict until now. AEM reveals complex behavior in DL.
<b>Large-scale Optimization (LSO) of multi-component electrolytes</b>	When chosen as an option, LSO performs calculations over matrices of electrolyte formulations to determine optimized values to achieve best performance under the optimization metrics (e.g., conductivity).	Greatly reduces time to identify optimized formulations and their performance and reduces laboratory measurements.

Quantity	Definition/Description	Importance and Application Areas
<b>Walden Parameters</b>	Walden terms shed light on the true interplay between viscosity and ionic conductivity in electrolytes.	The x and y axes for Walden plots are given in one of the output reports, covering each condition of temperature, solvent composition and salt concentration.
<b>Preferential Ion Solvation</b>	This metric considers the probability of finding each particular solvent in near proximity to an ion, given a solvent mixture. Covers both cation and anion species.	Preferential solvation is important to describing the solvation shell occupancy of ions. This matters, for example in effective solvated ion sizes, during early-life SEI formation processes and also as cells become polarized during operation.
<b>Cation Velocity over a range of potential gradients,</b>	The range of velocities of cation species in a battery determines how well power delivery can be sustained. It is a function of the electrolyte transport properties and the imposed potential gradient driving force.	These terms allow consideration of some concentration polarization (CP) effects. CP causes detrimental changes in electrolyte properties in double-layer regions.
<b>Solvent diffusion velocity</b>		
<b>Both are f(conc., T)</b>	Solvent diffusion velocity determines how readily solvent can back-diffuse after it is Faradaically carried with the cation or anion.	Electrolytes with higher velocities over a larger salt concentration range will be less prone toward CP development and related CP impedance increases.

Quantity	Definition/Description	Importance and Application Areas
<b>Surface Tension</b>	Surface tension reflects the cohesive energy an electrolyte has within itself. In AEM surface tension is calculated as a function of solvent mixture, salt concentration, and temperature.	Surface tension is a key parameter for looking at liquid permeation into porous media, where there exists both cohesive and adhesive (liquid-to-solid) considerations under competition.
<b>Electrolyte Migration into Porous Media</b>	This set of metrics considers the behavior of electrolyte migration into pores of a given dimension (diameter and length) and roughness. The user is queried to input the anticipated pore-related contact angle and other key terms.	Together with electrolyte properties (e.g., surface tension, viscosity, density, etc.) real porous media attributes will influence the rate of liquid infiltration. This is a key consideration for the wetting of porous solids and the effective liquid migration rates into porous structures having a wide range of dimensions.
<b>Solvent Activity</b>	Thermodynamic indicator of solvent availability, or conversely, indicator of solvent unavailability.	Ion solvation will diminish solvent activity, more so at higher salt conc. Important metric for SEI and HCE.
<b>Ligand-wise cation desolvation energy and time</b>	These terms represent the energy and kinetic requirements of solvent-wise removal from solvated cations.	Cation desolvation is a foremost consideration for applications that much achieve a bare cation in one or more processing steps.

**IMPORTANT NOTE:** There are additional output quantities that are found in the report files.

### **7.1.2 Data Output Reports and Definition of Terms**

◆ **Report1 -- Summary of Key Properties**

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)
wt fr salt (2)	weight fraction salt in electrolyte
mole fr salt	mole fraction salt in electrolyte
density (g/cc)	electrolyte density
visc. (cP)	electrolyte viscosity
sig1 (eff)	solvated cation diameter, effective Stokes transport basis, Angstroms
sig2 (eff)	solvated anion diameter, effective Stokes transport basis, Angstroms
S(+)	cation solvation number
Rational Act. Coef. y+/-	electrolyte salt activity coefficient, rational (molar) basis
Diff. Coeff. (cm^2/s)	diffusion coefficient or diffusivity for salt in electrolyte
Spec. Cond. (mS/cm)	specific conductivity of electrolyte
t+ (a)	cation transference number based on SI cations vs all charged species
t+ (b)	cation transference number based on all cation-bearing charged species vs all charged species
dissoc (SI)	fraction of salt dissociated into free single ions
dissoc (TI)	fraction of salt dissociated into triple ions

◆ **Report2 -- Ion association populations and other thermodynamic terms**

m2	molal salt conc.
c2	molar salt conc.
cmeff	effective molar concentration of all charged species
alphanet	total molar fraction of salt utilized in producing charged species
cation	mole fraction salt existing as cations
anion	mole fraction salt existing as anions
IP	mole fraction salt existing as ion pairs
TI	mole fraction salt existing as triple ions
fcip	fraction of ion pairs that are contact-type ion pairs
gamma+/-	molal-scale salt activity coefficient
y+/-	molar-scale salt activity coefficient
y+/-bar	molar-scale salt activity coefficient, using ion-averaged properties
Osmotic Coeff. (m)	Osmotic coefficient, molal basis
Osmotic Coeff. (M)	Osmotic coefficient, molar basis
Solvent Activity	Fraction of solvent "available" for associative and reactive processes
Kip	Ion Pair association equilibrium constant
Kti	Triple Ion association equilibrium constant
Ksol	Solid solvate association equilibrium constant

## Advanced Electrolyte Model (AEM)

### ◆ Report3 -- Ion solvation energies, permittivity and cation desolvation

m/c	molal/molar salt conc.
GFE cation	Gibbs free energy of cation solvation based on integral form
GFE anion	Gibbs free energy of anion solvation based on integral form
Solvation E, cation	cation solvation (binding) energy based on cation solvation number at salt conc.
Solvation E, anion	anion solvation (binding) energy based on anion solvation number at salt conc.
Rel. Permittivity, solution	relative permittivity for entire electrolyte solution
Rel. Permittivity, solvent	relative permittivity for electrolyte solvent mixture only
alpha1	fraction of salt dissociated into single (non-associated) ions
alpha3	fraction of salt dissociated into triple ions
Cation Desolv. Energy Sum	Ligand-wise summation of cation desolvation energies
Cation Desolv. Energy Ave	Ligand-wise average of cation desolvation energies
Cation Desolv. t	Ligand-wise summation of cation desolvation times

### ◆ Report4 -- Diffusivities and selected conductivity terms

m2	molal salt conc.
volsoft	volume fraction of solvent disrupted by ionic fields but not becoming solvators
fcomp	compression of solvent species in solvation shells relative to a reference molar volume at the same composition
fsolv	factor representing solvent-ion interactions that impact conductivity, akin to dielectric drag of solvent dipole(s) on ionic migration
fdiff12	factor covering the counter-ion geometric effects of ion transport, here for how the anion affects cation conductivity
D(+)	solvated cation diffusivity
D(-)	solvated anion diffusivity
D(-),bare*	bare anion diffusivity
DNernst	salt diffusivity according to the Nernst-type stoichiometric average
Dapp**	apparent salt diffusivity by applying the thermodynamic factor (akin to Newman value)
D(IP)	ion pair diffusivity
D(TI)	triple ion diffusivity
D(solvent)	solvent diffusivity
Thermodynamic Factor	Newman-type factor that is applied to DNernst to account for colligative thermodynamic effects

## Advanced Electrolyte Model (AEM)

### ◆ Report5 -- Summary of Transport Properties and Walden analysis

m2	molal salt conc.
c2	molar salt conc.
c2,pseudo	pseudo-molar salt concentration (moles per liter pure solvent)
density (g/cc)	electrolyte density
visc. (cP)	electrolyte viscosity
Rational Act. Coef. y+/-	electrolyte salt activity coefficient, rational (molar) basis
Diff. Coeff. (cm^2/s)	diffusion coefficient or diffusivity for salt in electrolyte
Spec. Cond. (mS/cm)	specific conductivity of electrolyte
t+ (a)	cation transference number based on SI cations vs all charged species
t+ (b)	cation transference number based on all cation-bearing charged species vs all charged species
fhop (+)	quantity that represents the relative prevalence of bare cation hoping as a cationic conduction mechanism, as defined over the conductive path length
fhop (-)	quantity that represents the relative prevalence of bare anion hoping as a anionic conduction mechanism, as defined over the conductive path length
Pos	Osmotic pressure in atmosphere units
Walden x	$\log(1/\text{visc})$ is used as the x axis for Walden-type plots
Walden y	$\log(\text{cond.})$ is used as the y axis for Walden-type plots; note that "cond." is conductance
Walden Product	product of electrolyte conductance times viscosity

### ◆ Report6 -- Activation Energies

salt molality	moles salt per kg pure solvent
1/visc	inverse viscosity
k*t+	product of specific conductivity times cation transference number
Diffusivity	diffusivity of salt in electrolyte (Nernst basis as in Report4)
Li-step (full)	Lithium Solvation and Transport Electrolyte Parameter, full form*
Li-step (solv.)	Lithium Solvation and Transport Electrolyte Parameter, solvation terms-only form*
Kip	Ion Pair association equilibrium constant
Kti	Triple Ion association equilibrium constant
Ksolv	Solid solvate association equilibrium constant
Solvent Activity	Fraction of solvent "available" for associative and reactive processes
gamma+/-	molal-scale salt activity coefficient

### ◆ **Report7 -- Large-Scale Simulation Optimization**

Output quantities for Report7 are self-explanatory. Note that both mole and mass fractions are used in reporting within Report7.

### ◆ **Report8 -- Non-convergent cases**

Non-convergent cases will be listed between the temperature and compositional legends. Non-convergent notations are generally of two types:

- '\*\*' If MSA-type chemical physics calculations or equilibrium determinations do not converge,
- Permittivity notification if solution or solvent permittivity calculations do not converge.

Upon non-convergence, the best information available at that point is utilized for remaining AEM calculations. If all cases converge between two temperatures, there will be no such notations.

### ◆ **Report9 -- Double-Layer Regions transport analysis**

The main tables generated in this report are defined with three regions of interest:

- Transport Region for Releasing Electrode (anode if discharge conditions, cathode if charge conditions)
- Separator Region
- Transport Region for Receiving Electrode (anode if charge conditions, cathode if discharge conditions)

Each table is printed at a particular elapsed time from the beginning of the charge or discharge event.

x	distance from the Releasing Electrode surface, Angstroms
C+	cation molar concentration at each x position
C-	anion molar concentration at each x position
Cs	solvent molar concentration at each x position
I	current at each x position, A
R	resistance at each x position, Ohm
ns+	cation solvation number at each x
ns-	anion solvation number at each x
v+	cation transport velocity at each x
v-	anion transport velocity at each x
dens.	electrolyte density at each x
visc.	electrolyte viscosity at each x
eff. cond.	effective electrolyte conductivity at the conditions of each x
t+	cation transference number at each x
'other'	generally refers to factors related to ionic hopping by cations and anions

## Advanced Electrolyte Model (AEM)

### ◆ Report10 -- Electrode surface-charge effects

Calculations are done at each temperature, covering a matrix of Surface Charge Densities at the target (cation receiving) electrode surface. Each temperature is considered since involved properties such as electrolyte permittivity are f(T).

r	distance from target electrode surface, Angstroms
Eff Surface Ch Density at r	effective surface charge density at r due to electron population
Solution Rel. Perm.	Solution relative permittivity at r as determined from electrolyte ionic and surface charge
Ave.(r) Solution Rel. Perm.	Solution relative permittivity averaged over r as determined from electrolyte ionic and surface charge
Electric Field per SCh	electric field at r as driven by the surface charge density of electrons
Repulsive Energy	repulsive energy over r between electrode surface charge density and averaged negative solvent dipole charge.
Cell Voltage	local voltage over r in response to surface charge effects, based on assumed starting cell voltage.

### ◆ Report11 -- Summary of Ion Solvation Quantities

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)
cation eff dia.	solvated cation diameter, effective Stokes transport basis, Angstroms
anion eff dia.	solvated anion diameter, effective Stokes transport basis, Angstroms
S <sub>+</sub> (th)	cation solvation number, thermodynamic basis
S <sub>-</sub> (th)	anion solvation number, thermodynamic basis
Solvent Avail. (thermo.)	free solvent availability based on subtraction of thermodynamically determined solvation numbers
Solvent Avail. (MSA HS)	free solvent availability based on subtraction of solvation numbers calculated from MSA hard-sphere solvated ion diameters
Solvent BE to cation	solvent binding energy to cation for energy minimized (equilibrium) cation solvation states.
Solvent BE to anion	solvent binding energy to anion for energy minimized (equilibrium) anion solvation states.
Communal Solvation Factor	(1 – CS factor) describes the relative likelihood of solvent being shared as a solvator between two or more charged species.
Debye Relaxation Time	approximate time for solvent to recover or relax its position (orientation) after being in proximity to a local ionic field, nanoseconds
Fraction of Free Liquid in Solvent	Solvents with higher melting points will have complex phase behavior in relation to electrolyte salt content. This term estimates the fraction of solvent that exists as liquid under (c,T) conditions. This impacts the effective electrolyte viscosity and related transport properties. The intended target is electrolytes with a single solvent having a melting point above 0 °C.

◆ Report12 -- Preferential Ion Solvation

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)

Other terms are self-explanatory. Results are provided for both the cation and anion, considering up to five solvents.

◆ Report13 -- Conductivity Factors

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)

Other terms are self-explanatory. Values shown are factors as applied to the modified Stokes expression for specific ionic conductivity. Results are provided for both the cation and anion, considering the seven conductivity factors mentioned in: [K. L Gering, Prediction of electrolyte conductivity: results from a generalized molecular model based on ion solvation and a chemical physics framework, Electrochim. Acta 225 \(2017\) 175–189.   
http://dx.doi.org/10.1016/j.electacta.2016.12.083.](#)

◆ Report14 -- Li-STEP Terms

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)

Other terms are explained below. Higher values of Li-STEP are desirable.

$$\begin{aligned}
 Li - STEP &= \frac{\kappa t_+}{\Delta t_{Li^+ desolv.}} \left[ \frac{\overline{BE}_{Li^+}}{RT} \right]^{-n_{s,Li^+}} \\
 &\simeq \kappa t_+ \left[ \frac{\overline{BE}_{Li^+}}{RT} \bar{\tau}_{Li^+} \right]^{-n_{s,Li^+}}
 \end{aligned}$$

### Lithium Solvation and Transport Electrolyte Parameter (Li-STEP)

Key transport and solvation terms are combined in a single parameter:

$$\text{Li-STEP} = \kappa t_+ \left[ \frac{\overline{\text{BE}}_{\text{Li}^+}}{RT} \bar{\tau}_{\text{Li}^+} \right]^{-n_{s,\text{Li}^+}}$$

The inverse of this quantity is akin to an impedance term for  $\text{Li}^+$  transport.

Parameter	Solvation component	Justification
Conductivity ( $\kappa$ )		Key Transport Parameter
Average Binding Energy ( $\overline{\text{BE}}_{\text{Li}^+}$ )		Thermodynamics of $\text{Li}^+$ solvation
Average solvent residence time ( $\bar{\tau}_{\text{Li}^+}$ )		Kinetics of $\text{Li}^+$ desolvation
Cation solvation number ( $n_{s,\text{Li}^+}$ )		Extent of $\text{Li}^+$ solvation
Cation transference number ( $t_+$ )		Efficiency of Lithium transport

Note:  $\overline{\text{BE}}_{\text{Li}^+}$  is a geometric average over all constituent ligands that comprise the cation solvation number. Thus, step-wise  $\text{Li}^+$  desolvation is described.  $n_{s,\text{Li}^+}$  is derived by a method adapted from Stokes and Robinson (1973).

*This new approach enables us to judge the relative contribution of each parameter to the overall activation energy of lithium transport, and leads to intelligent selection of electrolyte systems for high-power applications.*

#### ◆ Report15 -- Cation transit under Faradaic conditions

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)
v1	cation transit velocity, cm/s
t1	cation transit time between electrodes (assuming no polarization), s
vsolv	solvent transit velocity (determined from solvent diffusion migration rates), cm/s
tsolv	solvent transit time between electrodes (assuming no polarization), s
dV/dx	potential gradient, V/cm

#### ◆ Report16 -- Surface Tension and pore filling time over salt conc.

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)

Other terms are self-explanatory.

#### ◆ Report17 -- Percent pore length filled over time

Output terms are self-explanatory. Note that the time scale and time values (left-most column) may change between temperatures.

## Advanced Electrolyte Model (AEM)

### ◆ Report18 -- Ligand-wise cation desolvation energy and time

Herein, cation desolvation occurs in order of descending ligands: ....**BE5 → BE4 → BE3 → BE2 → BE1 → bare cation**, where the numbers represent quantity of solvators as determined through cation solvation numbers. Up to six ligands per cation are covered.

m2	molal salt conc. (moles salt per kg pure solvent)
c2	molar salt conc. (moles salt per liter electrolyte)
BE1....BE6	ligand-wise binding energy between solvent and cation, kJ/mole
BE, sum	summation of ligand-wise binding energies for cation, kJ/mole
dt1....dt6	ligand-wise desolvation time between solvent and cation, ns
dt, sum	summation of ligand-wise desolvation times for cation, ns
t-lambda	bulk screening term that reflects the many parameters that affect the cation desolvation process at an electrode interface and behavior of the local solvent population. The "Best" value is where t-lambda is minimized, indicating favorable conditions for cation desolvation and removal of shed solvent. t-lambda has units of ns.

### ◆ Report19 -- Ligand-wise cation desolvation energy and time (accounting for CS)

The output terms for this report are the same as for Report18, except the results account for the effects from Communal Ion Solvation (CS). That is, results are for cations in the CS-affected fraction of electrolyte.

### ◆ Report20 -- Terms relating to structure and Communal Ion Solvation (CS)

This report gives quantities that pertain to microstate structure in electrolytes. Two general factors contribute to structure beyond simple single-ion solvation: (1) communal solvation, CS (e.g., multidentate bridging) and (2) ion association (IA) and related solvation of IA species.

m2,bulk	bulk molal salt conc.
m2,non-CS	portion of molal salt conc. not involved in CS, i.e. simple single-ion solvation
m2,CS	portion of molal salt conc. involved in CS
y,free	fraction of solvent as free solvent (not participating as ion solvators)
y,non-CS	fraction of solvent participating in simple single-ion solvation
y,CS	fraction of solvent participating in CS
CS factor	communal solvation factor, probability that solvent is participating in CS
n,s+,bulk	cation solvation number in bulk electrolyte
n,s+,CS	cation solvation number in CS region
n,s+,ave	proportional average of n,s+,bulk and n,s+,CS
BE,+,bulk	solvent-to-cation binding energy in bulk electrolyte
BE,+,CS	solvent-to-cation binding energy in CS region
BE,+,ave	proportional average of BE,+,bulk and BE,+,CS
n,s,CS,0	bulk solvation number in CS region, baselined to CS with no IA
n,s,CS,ave	bulk solvation number in CS region, averaged over CS+IA
n,s,nonCS	bulk solvation number in non-CS region

## 7.2 AEM ACCC Solvent Class Examples

Edit ACCC Solvent Class

DMC      1

1. Solvent Class Name    2. Number of Solvents

Sol1

dimethyl carbonate	
3. Solvent 1 Identifier	
4. Molecular Weight 90.08 g/mole	5. Reference Temperature For Density 25. °C
6. Density at Reference Temperature 1.063 kg/L	7. Reference Temperature for Relative Permittivity 20. °C
8. Relative Permittivity at Reference Temperature 3.3	9. Parameter Related to the Temperature Dependence of Relative Permittivity -3.45e-03
10. Reference Temperature for Viscosity 25. °C	11. Viscosity at Reference Temperature 0.59 cP
12. Parameter Related to the Temperature Dependence of Viscosity 460.	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations 2.
14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt 1.12 ns	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C 0.47 ns
16. Variable for Solvated Cation Reference Ligand Length 6.56 nm	17. Variable for Solvated Ion 0.
18. Refractive Index (Na D line) 1.368	19. Dipole Moment, debye 0.93 D
20. π* Solvatochromic parameter 0.5	21. Reichardt's Normalized Polarity Index [E <sub>T,N</sub> ] 0.232
22. Reference Solvation Number for Cation at Infinite Dilution (estimate) 2.5	23. Reference Solvation Number for Anion at Infinite Dilution (estimate) 2.
24. Donicity or Gutmann Donor Number 17.5	25. Index for Solvent Solvation Configuration Around Cation 8
26. Index for Solvent Solvation Configuration Around Anion 8	27. Parameter for Solvent Solvation Configuration Around Cation 1.4
28. Parameter for Solvent Solvation Configuration Around Anion 1.57	29. Number of Atoms in Solvent Molecule 12
30. Classification for Configurational Entropy Calculations as Related to Surface Tension 1	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion 3.
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension 2.	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension 2.
34. Default Factor for Configurational Entropy, as Related to Surface Tension 1.	35. Index for Solvent Viscosity Mixing Rule 1

Save    Close

**Figure 155. ACCC Solvent Definition for DMC.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

DME	1
1. Solvent Class Name	2. Number of Solvents
<b>Sol1</b>	
1,2 dimethoxyethane	
3. Solvent 1 Identifier	
90.12 g/mole	4. Molecular Weight
25.	5. Reference Temperature For Density
0.86125 kg/L	6. Density at Reference Temperature
25.	7. Reference Temperature for Relative Permittivity
7.154	8. Relative Permittivity at Reference Temperature
-3.85e-03	9. Parameter Related to the Temperature Dependence of Relative Permittivity
25.	10. Reference Temperature for Viscosity
0.41 cP	11. Viscosity at Reference Temperature
380.	12. Parameter Related to the Temperature Dependence of Viscosity
2.	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations
1.	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt
0.3 ns	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C
6.1 nm	16. Variable for Solvated Cation Reference Ligand Length
0.	17. Variable for Solvated Ion
1.378	18. Refractive Index (Na D line)
1.61 D	19. Dipole Moment, debye
0.53	20. $\pi^*$ Solvatochromic parameter
0.231	21. Reichardt's Normalized Polarity Index [E <sub>T</sub> <sup>N</sup> ]
2.	22. Reference Solvation Number for Cation at Infinite Dilution (estimate)
1.25	23. Reference Solvation Number for Anion at Infinite Dilution (estimate)
18.4	24. Donicity or Gutmann Donor Number
7	25. Index for Solvent Solvation Configuration Around Cation
2	26. Index for Solvent Solvation Configuration Around Anion
2.4	27. Parameter for Solvent Solvation Configuration Around Cation
1.5	28. Parameter for Solvent Solvation Configuration Around Anion
16	29. Number of Atoms in Solvent Molecule
1	30. Classification for Configurational Entropy Calculations as Related to Surface Tension
2.	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion
4.	32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension
1.	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension
1.	34. Default Factor for Configurational Entropy, as Related to Surface Tension
3	35. Index for Solvent Viscosity Mixing Rule

Save      Close

**Figure 156. ACCC Solvent Definition for DME.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

EC	1.	2.
1. Solvent Class Name      2. Number of Solvents		
<b>Sol1</b>		
ethylene carbonate      3. Solvent 1 Identifier		
4. Molecular Weight	39.      °C	1.3214      kg/L
88.06      g/mole	-5.175e-03	40.      °C
5. Reference Temperature For Density      6. Density at Reference Temperature		
8. Relative Permittivity at Reference Temperature	9. Parameter Related to the Temperature Dependence of Relative Permittivity	10. Reference Temperature for Viscosity
90.36	-1.93	11. Viscosity at Reference Temperature
12. Parameter Related to the Temperature Dependence of Viscosity		
800.	1.5	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations
14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt		
16. Variable for Solvated Cation Reference Ligand Length	0.357      ns	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C
7.03      nm	0.      ns	16. Dipole Moment, debye
17. Variable for Solvated Ion		
19. Refractive Index (Na D line)	1.42	20. π* Solvatochromic parameter
20. π* Solvatochromic parameter	0.552      21. Reichardt's Normalized Polarity Index [ $E_7^N$ ]	22. Reference Solvation Number for Cation at Infinite Dilution (estimate)
24. Donicity or Gutmann Donor Number	10      25. Index for Solvent Solvation Configuration Around Cation	26. Index for Solvent Solvation Configuration Around Anion
16.4	10	27. Parameter for Solvent Solvation Configuration Around Cation
28. Parameter for Solvent Solvation Configuration Around Anion		
1.22	10      29. Number of Atoms in Solvent Molecule	30. Classification for Configurational Entropy Calculations as Related to Surface Tension
31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion		
3.      32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	0.      33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	1.      34. Default Factor for Configurational Entropy, as Related to Surface Tension
35. Index for Solvent Viscosity Mixing Rule		

**Figure 157. ACCC Solvent Definition for EC.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

EC_DMC_NPA	①	3	①
1. Solvent Class Name		2. Number of Solvents	
<b>Sol1      Sol2      Sol3</b>			
<input style="width: 100%; border: 1px solid #ccc; border-radius: 5px; padding: 2px;" type="text" value="ethylene carbonate"/> ① 3. Solvent 1 Identifier			
88.06	g/mole ①	39.	°C ①
4. Molecular Weight		5. Reference Temperature For Density	6. Density at Reference Temperature
1.93	kg/L ①	40.	°C ①
7. Reference Temperature for Relative Permittivity		8. Relative Permittivity at Reference Temperature	9. Parameter Related to the Temperature Dependence of Relative Permittivity
1.93	cP ①	10. Reference Temperature for Viscosity	11. Viscosity at Reference Temperature
800.	1.93	12. Parameter Related to the Temperature Dependence of Viscosity	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations
0.286	ns ①	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C
7.03	nm ①	16. Variable for Solvated Cation Reference Ligand Length	17. Variable for Solvated Ion
1.42	ns ①	18. Refractive Index (Na D line)	19. Dipole Moment, debye
0.84	0.552	20. π* Solvatochromic parameter	21. Reichardt's Normalized Polarity Index [E <sub>T</sub> <sup>N</sup> ]
1.28	1.28	22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	23. Reference Solvation Number for Anion at Infinite Dilution (estimate)
16.4	10	24. Donicity or Gutmann Donor Number	25. Index for Solvent Solvation Configuration Around Cation
2.0	2	26. Index for Solvent Solvation Configuration Around Anion	27. Parameter for Solvent Solvation Configuration Around Cation
1.22	10	28. Parameter for Solvent Solvation Configuration Around Anion	29. Number of Atoms in Solvent Molecule
3.	1	30. Classification for Configurational Entropy Calculations as Related to Surface Tension	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	0.	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	34. Default Factor for Configurational Entropy, as Related to Surface Tension
1	1	35. Index for Solvent Viscosity Mixing Rule	

**Figure 158. ACCC Solvent Definition for EC-DMC-NPA.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

1. Solvent Class Name <input type="text" value="EC_EMU"/>	2. Number of Solvents <input type="text" value="2"/>																																		
<p><b>Sol1</b>      <b>Sol2</b></p> <table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td colspan="2" style="text-align: center; padding-bottom: 5px;">3. Solvent 1 Identifier <input type="text" value="ethylene carbonate"/></td> </tr> <tr> <td style="width: 25%;">4. Molecular Weight <input type="text" value="88.06"/></td> <td style="width: 25%;">5. Reference Temperature For Density <input type="text" value="39."/></td> <td style="width: 25%;">6. Density at Reference Temperature <input type="text" value="1.3214"/></td> <td style="width: 25%;">7. Reference Temperature for Relative Permittivity <input type="text" value="40."/></td> </tr> <tr> <td>8. Relative Permittivity at Reference Temperature <input type="text" value="90.36"/></td> <td>-5.175e-03 <input type="text" value="9. Parameter Related to the Temperature Dependence of Relative Permittivity"/></td> <td>10. Reference Temperature for Viscosity <input type="text" value="40."/></td> <td>11. Viscosity at Reference Temperature <input type="text" value="1.93"/></td> </tr> <tr> <td>12. Parameter Related to the Temperature Dependence of Viscosity <input type="text" value="800."/></td> <td>13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations <input type="text" value="1.5"/></td> <td>14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt <input type="text" value="0.357"/></td> <td>15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C <input type="text" value="0.286"/></td> </tr> <tr> <td>16. Variable for Solvated Cation Reference Ligand Length <input type="text" value="7.03"/></td> <td>17. Variable for Solvated Ion <input type="text" value="0."/></td> <td>18. Refractive Index (Na D line) <input type="text" value="1.42"/></td> <td>19. Dipole Moment, debye <input type="text" value="4.51"/></td> </tr> <tr> <td>20. <math>\pi^*</math> Solvatochromic parameter <input type="text" value="0.84"/></td> <td>21. Reichardt's Normalized Polarity Index <math>[E_7^N]</math> <input type="text" value="0.552"/></td> <td>22. Reference Solvation Number for Cation at Infinite Dilution (estimate) <input type="text" value="4."/></td> <td>23. Reference Solvation Number for Anion at Infinite Dilution (estimate) <input type="text" value="1."/></td> </tr> <tr> <td>24. Donicity or Gutmann Donor Number <input type="text" value="16.4"/></td> <td>25. Index for Solvent Solvation Configuration Around Cation <input type="text" value="10"/></td> <td>26. Index for Solvent Solvation Configuration Around Anion <input type="text" value="2"/></td> <td>27. Parameter for Solvent Solvation Configuration Around Cation <input type="text" value="1.28"/></td> </tr> <tr> <td>28. Parameter for Solvent Solvation Configuration Around Anion <input type="text" value="1.22"/></td> <td>29. Number of Atoms in Solvent Molecule <input type="text" value="10"/></td> <td>30. Classification for Configurational Entropy Calculations as Related to Surface Tension <input type="text" value="1"/></td> <td>31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion <input type="text" value="3."/></td> </tr> <tr> <td>32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension <input type="text" value="3."/></td> <td>33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension <input type="text" value="0."/></td> <td>34. Default Factor for Configurational Entropy, as Related to Surface Tension <input type="text" value="1."/></td> <td>35. Index for Solvent Viscosity Mixing Rule <input type="text" value="1"/></td> </tr> </table>		3. Solvent 1 Identifier <input type="text" value="ethylene carbonate"/>		4. Molecular Weight <input type="text" value="88.06"/>	5. Reference Temperature For Density <input type="text" value="39."/>	6. Density at Reference Temperature <input type="text" value="1.3214"/>	7. Reference Temperature for Relative Permittivity <input type="text" value="40."/>	8. Relative Permittivity at Reference Temperature <input type="text" value="90.36"/>	-5.175e-03 <input type="text" value="9. Parameter Related to the Temperature Dependence of Relative Permittivity"/>	10. Reference Temperature for Viscosity <input type="text" value="40."/>	11. Viscosity at Reference Temperature <input type="text" value="1.93"/>	12. Parameter Related to the Temperature Dependence of Viscosity <input type="text" value="800."/>	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations <input type="text" value="1.5"/>	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt <input type="text" value="0.357"/>	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C <input type="text" value="0.286"/>	16. Variable for Solvated Cation Reference Ligand Length <input type="text" value="7.03"/>	17. Variable for Solvated Ion <input type="text" value="0."/>	18. Refractive Index (Na D line) <input type="text" value="1.42"/>	19. Dipole Moment, debye <input type="text" value="4.51"/>	20. $\pi^*$ Solvatochromic parameter <input type="text" value="0.84"/>	21. Reichardt's Normalized Polarity Index $[E_7^N]$ <input type="text" value="0.552"/>	22. Reference Solvation Number for Cation at Infinite Dilution (estimate) <input type="text" value="4."/>	23. Reference Solvation Number for Anion at Infinite Dilution (estimate) <input type="text" value="1."/>	24. Donicity or Gutmann Donor Number <input type="text" value="16.4"/>	25. Index for Solvent Solvation Configuration Around Cation <input type="text" value="10"/>	26. Index for Solvent Solvation Configuration Around Anion <input type="text" value="2"/>	27. Parameter for Solvent Solvation Configuration Around Cation <input type="text" value="1.28"/>	28. Parameter for Solvent Solvation Configuration Around Anion <input type="text" value="1.22"/>	29. Number of Atoms in Solvent Molecule <input type="text" value="10"/>	30. Classification for Configurational Entropy Calculations as Related to Surface Tension <input type="text" value="1"/>	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion <input type="text" value="3."/>	32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension <input type="text" value="3."/>	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension <input type="text" value="0."/>	34. Default Factor for Configurational Entropy, as Related to Surface Tension <input type="text" value="1."/>	35. Index for Solvent Viscosity Mixing Rule <input type="text" value="1"/>
3. Solvent 1 Identifier <input type="text" value="ethylene carbonate"/>																																			
4. Molecular Weight <input type="text" value="88.06"/>	5. Reference Temperature For Density <input type="text" value="39."/>	6. Density at Reference Temperature <input type="text" value="1.3214"/>	7. Reference Temperature for Relative Permittivity <input type="text" value="40."/>																																
8. Relative Permittivity at Reference Temperature <input type="text" value="90.36"/>	-5.175e-03 <input type="text" value="9. Parameter Related to the Temperature Dependence of Relative Permittivity"/>	10. Reference Temperature for Viscosity <input type="text" value="40."/>	11. Viscosity at Reference Temperature <input type="text" value="1.93"/>																																
12. Parameter Related to the Temperature Dependence of Viscosity <input type="text" value="800."/>	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations <input type="text" value="1.5"/>	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt <input type="text" value="0.357"/>	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C <input type="text" value="0.286"/>																																
16. Variable for Solvated Cation Reference Ligand Length <input type="text" value="7.03"/>	17. Variable for Solvated Ion <input type="text" value="0."/>	18. Refractive Index (Na D line) <input type="text" value="1.42"/>	19. Dipole Moment, debye <input type="text" value="4.51"/>																																
20. $\pi^*$ Solvatochromic parameter <input type="text" value="0.84"/>	21. Reichardt's Normalized Polarity Index $[E_7^N]$ <input type="text" value="0.552"/>	22. Reference Solvation Number for Cation at Infinite Dilution (estimate) <input type="text" value="4."/>	23. Reference Solvation Number for Anion at Infinite Dilution (estimate) <input type="text" value="1."/>																																
24. Donicity or Gutmann Donor Number <input type="text" value="16.4"/>	25. Index for Solvent Solvation Configuration Around Cation <input type="text" value="10"/>	26. Index for Solvent Solvation Configuration Around Anion <input type="text" value="2"/>	27. Parameter for Solvent Solvation Configuration Around Cation <input type="text" value="1.28"/>																																
28. Parameter for Solvent Solvation Configuration Around Anion <input type="text" value="1.22"/>	29. Number of Atoms in Solvent Molecule <input type="text" value="10"/>	30. Classification for Configurational Entropy Calculations as Related to Surface Tension <input type="text" value="1"/>	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion <input type="text" value="3."/>																																
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension <input type="text" value="3."/>	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension <input type="text" value="0."/>	34. Default Factor for Configurational Entropy, as Related to Surface Tension <input type="text" value="1."/>	35. Index for Solvent Viscosity Mixing Rule <input type="text" value="1"/>																																

**Figure 159. ACCC Solvent Definition for EC-EMC.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

EC_PC_EMC_MA_BN	(i)	5	(i)
1. Solvent Class Name		2. Number of Solvents	
Sol1	Sol2	Sol3	Sol4
Sol5			
ethylene carbonate (i)			
3. Solvent 1 Identifier			
88.06	g/mole (i)	39.	°C (i)
4. Molecular Weight		5. Reference Temperature For Density	
1.3214	kg/L (i)	6. Density at Reference Temperature	
40.	°C (i)	7. Reference Temperature for Relative Permittivity	
90.36	(i)	-5.175e-03	(i)
8. Relative Permittivity at Reference Temperature		9. Parameter Related to the Temperature Dependence of Relative Permittivity	
40.	°C (i)	10. Reference Temperature for Viscosity	
1.93	cP (i)	11. Viscosity at Reference Temperature	
800.	(i)	1.5	(i)
12. Parameter Related to the Temperature Dependence of Viscosity		13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	
0.357	ns (i)	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	
0.286	ns (i)	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C	
7.03	nm (i)	0.	(i)
16. Variable for Solvated Cation Reference Ligand Length		17. Variable for Solvated Ion	
1.42	(i)	18. Refractive Index (Na D line)	
4.51	D (i)	19. Dipole Moment, debye	
0.84	(i)	0.552	(i)
20. π* Solvatochromic parameter		21. Reichardt's Normalized Polarity Index [E <sub>r</sub> <sup>N</sup> ]	
4.	(i)	22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	
1.28	(i)	23. Reference Solvation Number for Anion at Infinite Dilution (estimate)	
16.4	(i)	10	(i)
24. Donicity or Gutmann Donor Number		25. Index for Solvent Solvation Configuration Around Cation	
2.	(i)	26. Index for Solvent Solvation Configuration Around Anion	
1.22	(i)	1	(i)
28. Parameter for Solvent Solvation Configuration Around Anion		30. Classification for Configurational Entropy Calculations as Related to Surface Tension	
3.	(i)	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion	
0.	(i)	32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	
1.	(i)	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	
1.	(i)	34. Default Factor for Configurational Entropy, as Related to Surface Tension	
1	(i)	35. Index for Solvent Viscosity Mixing Rule	

**Figure 160. ACCC Solvent Definition for EC-PC-EMC-MA-BN.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

EMC	1
1. Solvent Class Name	
2. Number of Solvents	
<b>Sol1</b>	
ethylmethyl carbonate	
3. Solvent 1 Identifier	
4. Molecular Weight	104.11 g/mole
5. Reference Temperature For Density	25. °C
6. Density at Reference Temperature	1.007 kg/L
7. Reference Temperature for Relative Permittivity	25. °C
8. Relative Permittivity at Reference Temperature	2.958
9. Parameter Related to the Temperature Dependence of Relative Permittivity	-3.65e-03
10. Reference Temperature for Viscosity	25. °C
11. Viscosity at Reference Temperature	0.66 cP
12. Parameter Related to the Temperature Dependence of Viscosity	410.
13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	2.
14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	1.01 ns
15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C	0.45 ns
16. Variable for Solvated Cation Reference Ligand Length	6.936 nm
17. Variable for Solvated Ion	0.
18. Refractive Index (Na D line)	1.376
19. Dipole Moment, debye	1.0 D
20. $\pi^*$ Solvatochromic parameter	0.47
21. Reichardt's Normalized Polarity Index [ $E_1^{\text{N}}$ ]	0.21
22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	2.
23. Reference Solvation Number for Anion at Infinite Dilution (estimate)	2.
24. Donicity or Gutmann Donor Number	15.7
25. Index for Solvent Solvation Configuration Around Cation	8
26. Index for Solvent Solvation Configuration Around Anion	2
27. Parameter for Solvent Solvation Configuration Around Cation	1.3
28. Parameter for Solvent Solvation Configuration Around Anion	1.6
29. Number of Atoms in Solvent Molecule	15
30. Classification for Configurational Entropy Calculations as Related to Surface Tension	1
31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion	3.
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	3.
33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	3.
34. Default Factor for Configurational Entropy, as Related to Surface Tension	1
35. Index for Solvent Viscosity Mixing Rule	1

**Figure 161. ACCC Solvent Definition for EMC.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

EP	1		
1. Solvent Class Name			
2. Number of Solvents			
<b>Sol1</b>			
ethyl propionate <span style="font-size: small;">(i)</span>			
3. Solvent 1 Identifier			
4. Molecular Weight 102.13 g/mole <span style="font-size: small;">(i)</span>	5. Reference Temperature For Density 16. ${}^{\circ}\text{C}$ <span style="font-size: small;">(i)</span>	6. Density at Reference Temperature 0.895 kg/L <span style="font-size: small;">(i)</span>	
7. Reference Temperature for Relative Permittivity 25. ${}^{\circ}\text{C}$ <span style="font-size: small;">(i)</span>	8. Relative Permittivity at Reference Temperature 5.65 <span style="font-size: small;">(i)</span>	9. Parameter Related to the Temperature Dependence of Relative Permittivity -3.65e-03 <span style="font-size: small;">(i)</span>	
10. Reference Temperature for Viscosity 25. ${}^{\circ}\text{C}$ <span style="font-size: small;">(i)</span>	11. Viscosity at Reference Temperature 0.51 cP <span style="font-size: small;">(i)</span>	12. Parameter Related to the Temperature Dependence of Viscosity 520. <span style="font-size: small;">(i)</span>	
13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations 2. <span style="font-size: small;">(i)</span>	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 ${}^{\circ}\text{C}$ , Infinite Dilution Salt 0.9568 ns <span style="font-size: small;">(i)</span>	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 ${}^{\circ}\text{C}$ 0.3675 ns <span style="font-size: small;">(i)</span>	
16. Variable for Solvated Cation Reference Ligand Length 6.6 nm <span style="font-size: small;">(i)</span>	17. Variable for Solvated Ion 0. <span style="font-size: small;">(i)</span>	18. Refractive Index (Na D line) 1.381 <span style="font-size: small;">(i)</span>	19. Dipole Moment, debye 1.8 D <span style="font-size: small;">(i)</span>
20. $n^*$ Solvatochromic parameter 0.5 <span style="font-size: small;">(i)</span>	21. Reichardt's Normalized Polarity Index [E] <sub>N</sub> 0.25 <span style="font-size: small;">(i)</span>	22. Reference Solvation Number for Cation at Infinite Dilution (estimate) 2. <span style="font-size: small;">(i)</span>	23. Reference Solvation Number for Anion at Infinite Dilution (estimate) 1. <span style="font-size: small;">(i)</span>
24. Donicity or Gutmann Donor Number 16.7 <span style="font-size: small;">(i)</span>	25. Index for Solvent Solvation Configuration Around Cation 7. <span style="font-size: small;">(i)</span>	26. Index for Solvent Solvation Configuration Around Anion 6. <span style="font-size: small;">(i)</span>	27. Parameter for Solvent Solvation Configuration Around Cation 1.1 <span style="font-size: small;">(i)</span>
28. Parameter for Solvent Solvation Configuration Around Anion 1.85 <span style="font-size: small;">(i)</span>	29. Number of Atoms in Solvent Molecule 17. <span style="font-size: small;">(i)</span>	30. Classification for Configurational Entropy Calculations as Related to Surface Tension 1. <span style="font-size: small;">(i)</span>	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion 2. <span style="font-size: small;">(i)</span>
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension 5. <span style="font-size: small;">(i)</span>	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension 3. <span style="font-size: small;">(i)</span>	34. Default Factor for Configurational Entropy, as Related to Surface Tension 1. <span style="font-size: small;">(i)</span>	35. Index for Solvent Viscosity Mixing Rule 1. <span style="font-size: small;">(i)</span>

**Figure 162. ACCC Solvent Definition for EP.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

EP_BN	2		
1. Solvent Class Name      2. Number of Solvents			
<input checked="" type="radio"/> Sol1 <input type="radio"/> Sol2			
ethyl propionate      ⓘ 3. Solvent 1 Identifier			
4. Molecular Weight	16.      °C ⓘ	0.895      kg/L ⓘ	25.      °C ⓘ
5. Relative Permittivity at Reference Temperature	-3.65e-03	6. Density at Reference Temperature	7. Reference Temperature for Relative Permittivity
5.65	25.	0.895	0.51
12. Parameter Related to the Temperature Dependence of Viscosity	2.	kg/L	cP ⓘ
540.	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	ns	11. Viscosity at Reference Temperature
6.6	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	0.3	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C
16. Variable for Solvated Cation Reference Ligand Length	17. Variable for Solvated Ion	1.381	1.8
0.5	18. Refractive Index (Na D line)	D ⓘ	19. Dipole Moment, debye
20. $\pi^*$ Solvatochromic parameter	21. Reichardt's Normalized Polarity Index [E <sub>T</sub> <sup>N</sup> ]	2.	1.
16.7	22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	1.35	23. Reference Solvation Number for Anion at Infinite Dilution (estimate)
24. Donicity or Gutmann Donor Number	25. Index for Solvent Solvation Configuration Around Cation	6	27. Parameter for Solvent Solvation Configuration Around Cation
1.45	29. Number of Atoms in Solvent Molecule	1	2.
28. Parameter for Solvent Solvation Configuration Around Anion	30. Classification for Configurational Entropy Calculations as Related to Surface Tension	1.35	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion
5.	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	1.	35. Index for Solvent Viscosity Mixing Rule
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	34. Default Factor for Configurational Entropy, as Related to Surface Tension	1	

**Figure 163. ACCC Solvent Definition for EP-BN.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

MA	1		
1. Solvent Class Name      2. Number of Solvents			
X			
Sol1			
methyl acetate			
3. Solvent 1 Identifier			
4. Molecular Weight	25. Reference Temperature For Density	6. Density at Reference Temperature	20. Reference Temperature for Relative Permittivity
74.08 g/mole	°C	kg/L	°C
5. Parameter Related to the Temperature Dependence of Relative Permittivity		7. Relative Permittivity at Reference Temperature	
6.94	-4.1e-03	20.	0.381
8. Relative Permittivity at Reference Temperature		10. Reference Temperature for Viscosity	
400.	2.	°C	cP
12. Parameter Related to the Temperature Dependence of Viscosity		11. Viscosity at Reference Temperature	
6.16 nm	0.	ns	ns
16. Variable for Solvated Cation Reference Ligand Length		13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	
0.6	0.253	ns	ns
20. $\pi^*$ Solvatochromic parameter		14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	
17.7	7	ns	ns
24. Donicity or Gutmann Donor Number		15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C	
1.2	11	1.361	D
28. Parameter for Solvent Solvation Configuration Around Anion		18. Refractive Index (Na D line)	
3.	1.	1.69	D
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension		19. Dipole Moment, debye	
0.253	21. Reichardt's Normalized Polarity Index [ $E_T^N$ ]	2.5	1.5
25. Index for Solvent Solvation Configuration Around Cation		22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	
4	26. Index for Solvent Solvation Configuration Around Anion	1.56	1.56
28. Parameter for Solvent Solvation Configuration Around Anion		27. Parameter for Solvent Solvation Configuration Around Cation	
1	30. Classification for Configurational Entropy Calculations as Related to Surface Tension	2.	2.
1.	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion	1.	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion
1.	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	1.	35. Index for Solvent Viscosity Mixing Rule
1.	34. Default Factor for Configurational Entropy, as Related to Surface Tension	1	

**Figure 164. ACCC Solvent Definition for MA.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

NPA	1	X
1. Solvent Class Name	2. Number of Solvents	
<b>Sol1</b>		
n-propyl acetate		
3. Solvent 1 Identifier		
4. Molecular Weight	5. Reference Temperature For Density	6. Density at Reference Temperature
102.13 g/mole	25. °C	0.883 kg/L
8. Relative Permittivity at Reference Temperature	9. Parameter Related to the Temperature Dependence of Relative Permittivity	20. °C
480.	-3.85e-03	25. °C
12. Parameter Related to the Temperature Dependence of Viscosity	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	10. Reference Temperature for Viscosity
6.76 nm	2. ns	0.55 cP
16. Variable for Solvated Cation Reference Ligand Length	17. Variable for Solvated Ion	11. Viscosity at Reference Temperature
0.45	0.21	1.78 D
20. $\pi^*$ Solvatochromic parameter	21. Reichardt's Normalized Polarity Index [ $E_T^N$ ]	19. Dipole Moment, debye
15.7	7	1.1
24. Donicity or Gutmann Donor Number	25. Index for Solvent Solvation Configuration Around Cation	23. Reference Solvation Number for Cation at Infinite Dilution (estimate)
1.6	17	2.1
28. Parameter for Solvent Solvation Configuration Around Anion	29. Number of Atoms in Solvent Molecule	27. Parameter for Solvent Solvation Configuration Around Cation
5.	2.5	2.2
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion
1.	1.	1.
34. Default Factor for Configurational Entropy, as Related to Surface Tension	35. Index for Solvent Viscosity Mixing Rule	

**Figure 165. ACCC Solvent Definition for NPA.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

X

1. Solvent Class Name	2. Number of Solvents
PC	1
<b>Sol1</b>	
propylene carbonate <span style="font-size: small;">(i)</span>	
3. Solvent 1 Identifier	
4. Molecular Weight	102.09 g/mole <span style="font-size: small;">(i)</span>
5. Reference Temperature For Density	25. °C <span style="font-size: small;">(i)</span>
6. Density at Reference Temperature	1.199862 kg/L <span style="font-size: small;">(i)</span>
7. Reference Temperature for Relative Permittivity	25. °C <span style="font-size: small;">(i)</span>
8. Relative Permittivity at Reference Temperature	65.1848 <span style="font-size: small;">(i)</span>
9. Parameter Related to the Temperature Dependence of Relative Permittivity	-3.65e-03 <span style="font-size: small;">(i)</span>
10. Reference Temperature for Viscosity	25. °C <span style="font-size: small;">(i)</span>
11. Viscosity at Reference Temperature	2.54187 cP <span style="font-size: small;">(i)</span>
12. Parameter Related to the Temperature Dependence of Viscosity	830. <span style="font-size: small;">(i)</span>
13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	1.5 <span style="font-size: small;">(i)</span>
14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	0.47 ns <span style="font-size: small;">(i)</span>
15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C	0.67 ns <span style="font-size: small;">(i)</span>
16. Variable for Solvated Cation Reference Ligand Length	7.44 nm <span style="font-size: small;">(i)</span>
17. Variable for Solvated Ion	0. <span style="font-size: small;">(i)</span>
18. Refractive Index (Na D line)	1.4209 <span style="font-size: small;">(i)</span>
19. Dipole Moment, debye	4.98 D <span style="font-size: small;">(i)</span>
20. $\pi^*$ Solvatochromic parameter	0.83 <span style="font-size: small;">(i)</span>
21. Reichardt's Normalized Polarity Index [ $E_T^N$ ]	0.472 <span style="font-size: small;">(i)</span>
22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	4. <span style="font-size: small;">(i)</span>
23. Reference Solvation Number for Anion at Infinite Dilution (estimate)	2. <span style="font-size: small;">(i)</span>
24. Donicity or Gutmann Donor Number	15.1 <span style="font-size: small;">(i)</span>
25. Index for Solvent Solvation Configuration Around Cation	4 <span style="font-size: small;">(i)</span>
26. Index for Solvent Solvation Configuration Around Anion	4 <span style="font-size: small;">(i)</span>
27. Parameter for Solvent Solvation Configuration Around Cation	1.6 <span style="font-size: small;">(i)</span>
28. Parameter for Solvent Solvation Configuration Around Anion	0.65 <span style="font-size: small;">(i)</span>
29. Number of Atoms in Solvent Molecule	13 <span style="font-size: small;">(i)</span>
30. Classification for Configurational Entropy Calculations as Related to Surface Tension	2 <span style="font-size: small;">(i)</span>
31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion	3. <span style="font-size: small;">(i)</span>
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	4. <span style="font-size: small;">(i)</span>
33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	1. <span style="font-size: small;">(i)</span>
34. Default Factor for Configurational Entropy, as Related to Surface Tension	1. <span style="font-size: small;">(i)</span>
35. Index for Solvent Viscosity Mixing Rule	2 <span style="font-size: small;">(i)</span>

Save      Close

**Figure 166. ACCC Solvent Definition for PC**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

1. Solvent Class Name	PC_EC_EMC_MA_BN	2. Number of Solvents	5
Sol1 Sol2 Sol3 Sol4 Sol5			
propylene carbonate 3. Solvent 1 Identifier			
4. Molecular Weight	102.09 g/mole	5. Reference Temperature For Density	25. °C
6. Density at Reference Temperature	1.199862 kg/L	7. Reference Temperature for Relative Permittivity	25. °C
8. Relative Permittivity at Reference Temperature	65.1848	9. Parameter Related to the Temperature Dependence of Relative Permittivity	-3.65e-03
10. Reference Temperature for Viscosity	25. °C	11. Viscosity at Reference Temperature	25.4187 cP
12. Parameter Related to the Temperature Dependence of Viscosity	830.	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	1.5 ns
14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	0.47 ns	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C	0.67 ns
16. Variable for Solvated Cation Reference Ligand Length	7.44 nm	17. Variable for Solvated Ion	0. refractive index (Na D line)
18. Refractive Index (Na D line)	1.4209	19. Dipole Moment, debye	4.98 D
20. π* Solvatochromic parameter	0.83	21. Reichardt's Normalized Polarity Index [E <sub>T</sub> <sup>N</sup> ]	0.472
22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	4.	23. Reference Solvation Number for Anion at Infinite Dilution (estimate)	2.
24. Donicity or Gutmann Donor Number	15.1	25. Index for Solvent Solvation Configuration Around Cation	4.
26. Index for Solvent Solvation Configuration Around Anion	4.	27. Parameter for Solvent Solvation Configuration Around Cation	1.6
28. Parameter for Solvent Solvation Configuration Around Anion	0.65	29. Number of Atoms in Solvent Molecule	13.
30. Classification for Configurational Entropy Calculations as Related to Surface Tension	2.	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion	3.
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	4.	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	1.
34. Default Factor for Configurational Entropy, as Related to Surface Tension	1.	35. Index for Solvent Viscosity Mixing Rule	2.

**Figure 167. ACCC Solvent Definition for PC-EC-EMC-MA-BN.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

1. Solvent Class Name <b>PC_EMC</b>	2. Number of Solvents <b>2</b>		
<b>propylene carbonate</b> 3. Solvent 1 Identifier			
4. Molecular Weight <b>102.09 g/mole</b>	5. Reference Temperature For Density <b>25. °C</b>	6. Density at Reference Temperature <b>1.199862 kg/L</b>	7. Reference Temperature for Relative Permittivity <b>25. °C</b>
8. Relative Permittivity at Reference Temperature <b>65.1848</b>	9. Parameter Related to the Temperature Dependence of Relative Permittivity <b>-3.65e-03</b>	10. Reference Temperature for Viscosity <b>25. °C</b>	11. Viscosity at Reference Temperature <b>2.54187 cP</b>
12. Parameter Related to the Temperature Dependence of Viscosity <b>830.</b>	13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations <b>1.5</b>	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt <b>0.47 ns</b>	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C <b>0.67 ns</b>
16. Variable for Solvated Cation Reference Ligand Length <b>7.44 nm</b>	17. Variable for Solvated Ion <b>0.</b>	18. Refractive Index (Na D line) <b>1.4209</b>	19. Dipole Moment, debye <b>4.98 D</b>
20. $\pi^*$ Solvatochromic parameter <b>0.83</b>	21. Reichardt's Normalized Polarity Index [ $E_7^{N*}$ ] <b>0.472</b>	22. Reference Solvation Number for Cation at Infinite Dilution (estimate) <b>4.</b>	23. Reference Solvation Number for Anion at Infinite Dilution (estimate) <b>2.</b>
24. Donicity or Gutmann Donor Number <b>15.1</b>	25. Index for Solvent Solvation Configuration Around Cation <b>4</b>	26. Index for Solvent Solvation Configuration Around Anion <b>4</b>	27. Paramater for Solvent Solvation Configuration Around Cation <b>1.6</b>
28. Parameter for Solvent Solvation Configuration Around Anion <b>0.65</b>	29. Number of Atoms in Solvent Molecule <b>13</b>	30. Classification for Configurational Entropy Calculations as Related to Surface Tension <b>2</b>	31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion <b>3.</b>
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension <b>4.</b>	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension <b>1.</b>	34. Default Factor for Configurational Entropy, as Related to Surface Tension <b>1.</b>	35. Index for Solvent Viscosity Mixing Rule <b>2</b>

**Figure 168. ACCC Solvent Definition for PC-EMC.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

PN	1	
1. Solvent Class Name		
2. Number of Solvents		
<b>Sol1</b>		
propionitrile (PrN) <span style="font-size: small;">(i)</span>		
3. Solvent 1 Identifier		
4. Molecular Weight 55.08 g/mole <span style="font-size: small;">(i)</span>	5. Reference Temperature For Density 25. $^{\circ}\text{C}$ <span style="font-size: small;">(i)</span>	6. Density at Reference Temperature 0.777 kg/L <span style="font-size: small;">(i)</span>
7. Reference Temperature for Relative Permittivity 20. $^{\circ}\text{C}$ <span style="font-size: small;">(i)</span>	8. Relative Permittivity at Reference Temperature 28.86 <span style="font-size: small;">(i)</span>	9. Parameter Related to the Temperature Dependence of Relative Permittivity -4.3e-03 <span style="font-size: small;">(i)</span>
10. Reference Temperature for Viscosity 25. $^{\circ}\text{C}$ <span style="font-size: small;">(i)</span>	11. Viscosity at Reference Temperature 0.411 cP <span style="font-size: small;">(i)</span>	12. Parameter Related to the Temperature Dependence of Viscosity 580. <span style="font-size: small;">(i)</span>
13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations 0.27 ns <span style="font-size: small;">(i)</span>	14. Reference Value for Average Residence Time of Solvent Around Cation at 25 $^{\circ}\text{C}$ , Infinite Dilution Salt 0.62 ns <span style="font-size: small;">(i)</span>	15. Reference Value for Average Residence Time of Solvent Around Anion at 25 $^{\circ}\text{C}$ 0.27 ns <span style="font-size: small;">(i)</span>
16. Variable for Solvated Cation Reference Ligand Length 6.16 nm <span style="font-size: small;">(i)</span>	17. Variable for Solvated Ion 0. <span style="font-size: small;">(i)</span>	18. Refractive Index (Na D line) 1.366 <span style="font-size: small;">(i)</span>
19. Dipole Moment, debye 4.04 D <span style="font-size: small;">(i)</span>	20. $\pi^*$ Solvatochromic parameter 0.71 <span style="font-size: small;">(i)</span>	21. Reichardt's Normalized Polarity Index [ $E_7^N$ ] 0.398 <span style="font-size: small;">(i)</span>
22. Reference Solvation Number for Cation at Infinite Dilution (estimate) 1.5 <span style="font-size: small;">(i)</span>	23. Reference Solvation Number for Anion at Infinite Dilution (estimate) 1.6 <span style="font-size: small;">(i)</span>	24. Donicity or Gutmann Donor Number 16.1 <span style="font-size: small;">(i)</span>
25. Index for Solvent Solvation Configuration Around Cation 4 <span style="font-size: small;">(i)</span>	26. Index for Solvent Solvation Configuration Around Anion 14 <span style="font-size: small;">(i)</span>	27. Parameter for Solvent Solvation Configuration Around Cation 1.4 <span style="font-size: small;">(i)</span>
28. Parameter for Solvent Solvation Configuration Around Anion 1.45 <span style="font-size: small;">(i)</span>	29. Number of Atoms in Solvent Molecule 9 <span style="font-size: small;">(i)</span>	30. Classification for Configurational Entropy Calculations as Related to Surface Tension 1 <span style="font-size: small;">(i)</span>
31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion 1. <span style="font-size: small;">(i)</span>	32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension 3. <span style="font-size: small;">(i)</span>	33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension 1. <span style="font-size: small;">(i)</span>
34. Default Factor for Configurational Entropy, as Related to Surface Tension 1 <span style="font-size: small;">(i)</span>	35. Index for Solvent Viscosity Mixing Rule 1 <span style="font-size: small;">(i)</span>	

**Figure 169. ACCC Solvent Definition for PN.**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Solvent Class**

1. Solvent Class Name	2. Number of Solvents
X	
<b>Sol1</b>	
vinyl ethylene carbonate      ⓘ	
3. Solvent 1 Identifier	
4. Molecular Weight	114.0993 g/mole ⓘ
5. Reference Temperature For Density	20. °C ⓘ
6. Density at Reference Temperature	1.188 kg/L ⓘ
7. Reference Temperature for Relative Permittivity	25. °C ⓘ
8. Relative Permittivity at Reference Temperature	2.2 cP ⓘ
9. Parameter Related to the Temperature Dependence of Relative Permittivity	10. Reference Temperature for Viscosity
11. Viscosity at Reference Temperature	25. °C ⓘ
12. Parameter Related to the Temperature Dependence of Viscosity	11. Viscosity at Reference Temperature
13. Reference Maximum Solvation Sites Within a Single Solvent Molecule that Promote Interaction With Cations	2.2 ns ⓘ
14. Reference Value for Average Residence Time of Solvent Around Cation at 25 °C, Infinite Dilution Salt	0.55 ns ⓘ
15. Reference Value for Average Residence Time of Solvent Around Anion at 25 °C	0.6 ns ⓘ
16. Variable for Solvated Cation Reference Ligand Length	7. nm ⓘ
17. Variable for Solvated Ion	0. ns ⓘ
18. Refractive Index (Na D line)	1.546 ⓘ
19. Dipole Moment, debye	3.5 D ⓘ
20. π* Solvatochromic parameter	0.83 ⓘ
21. Reichardt's Normalized Polarity Index [E <sub>r</sub> <sup>N</sup> ]	0.51 ⓘ
22. Reference Solvation Number for Cation at Infinite Dilution (estimate)	4. ⓘ
23. Reference Solvation Number for Anion at Infinite Dilution (estimate)	2. ⓘ
24. Donicity or Gutmann Donor Number	15. ⓘ
25. Index for Solvent Solvation Configuration Around Cation	10. ⓘ
26. Index for Solvent Solvation Configuration Around Anion	4. ⓘ
27. Parameter for Solvent Solvation Configuration Around Cation	1.3 ⓘ
28. Parameter for Solvent Solvation Configuration Around Anion	1.35 ⓘ
29. Number of Atoms in Solvent Molecule	14 ⓘ
30. Classification for Configurational Entropy Calculations as Related to Surface Tension	1. ⓘ
31. Parameter for Oxygen (or S, P) Species in Configurational Entropy, as Related to Surface Tension Configuration Around Anion	4. ⓘ
32. Parameter for Carbon Species in Configurational Entropy, as Related to Surface Tension	2. ⓘ
33. Parameter for Molecular Pivot Points in Solvent for Configurational Entropy, as Related to Surface Tension	1. ⓘ
34. Default Factor for Configurational Entropy, as Related to Surface Tension	2. ⓘ
35. Index for Solvent Viscosity Mixing Rule	1. ⓘ

**Figure 170. ACCC Solvent Definition for VEC.**

## 7.3 AEM ACCC Salt Class Examples

**Edit ACCC Salt Class**

<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="LiBOB_w_PC_EA"/> Salt Class Name	<span style="font-size: 2em;">X</span>		
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="LiBOB"/> Salt Identifier			
<input checked="" type="radio"/> Regular Salt <input type="radio"/> Ionic Liquid			
<b>Salt Type</b>			
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="1.36"/> Diameter of Cation from Crystalline Basis Å	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="6.396"/> Diameter of Anion from Crystalline Basis Å	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="3.358"/> Equivalent Diameter of Anion Accounting for Electrostatic Charge Distribution of Anion Å	
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="1."/> Unit Charge of Cation	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="-1."/> Unit Charge of Anion	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="193.79"/> Molecular Weight of Salt g/mole	
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="1.62"/> Density of Pure Crystalline Salt g/cm <sup>3</sup>	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="19.3"/> Relative Permittivity of Pure Crystalline Salt		
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="2"/> Number of Solvents			
<b>Sol1</b> <b>Sol2</b>			
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="0.47"/> Average Residence Time of Solvent Around Cation ns	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="0.5"/> Average Residence Time of Solvent Around Anion ns	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="4."/> Cation Reference Solvation Number	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="2."/> Anion Reference Solvation Number
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="4"/> Index for Solvent Solvation Configuration Around Cation	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="4"/> Index for Solvent Solvation Configuration Around Anion	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="1.6"/> Parameter for Solvent Solvation Configuration Around Cation	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="2.8"/> Parameter for Solvent Solvation Configuration Around Anion
<a href="#">Save</a> <a href="#">Close</a>			

<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="0.9"/> Average Residence Time of Solvent Around Cation ns	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="0.38"/> Average Residence Time of Solvent Around Anion ns	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="2."/> Cation Reference Solvation Number	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="1.5"/> Anion Reference Solvation Number
<b>Sol1</b> <b>Sol2</b>			
<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="3"/> Index for Solvent Solvation Configuration Around Cation	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="4"/> Index for Solvent Solvation Configuration Around Anion	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="1.22"/> Parameter for Solvent Solvation Configuration Around Cation	<input style="border: 1px solid #ccc; padding: 2px; width: 100%;" type="text" value="4.2"/> Parameter for Solvent Solvation Configuration Around Anion
<a href="#">Save</a> <a href="#">Close</a>			

**Figure 171. ACCC Salt Definition for LiBOB\_w\_PC\_EA**

## Advanced Electrolyte Model (AEM)

**Edit ACCC Salt Class**

Salt Class Name

Salt Identifier

Regular Salt
Ionic Liquid

Diameter of Cation from Crystalline Basis

Diameter of Anion from Crystalline Basis [Å]

Equivalent Diameter of Anion Accounting for Electrostatic Charge Distribution of Anion

Number of Charge Regions for Anion

Unit Charge of Cation

Unit Charge of Anion

Molecular Weight of Salt

Molecular Weight of Cation

Density of Pure Crystalline Salt

Relative Permittivity of Pure Crystalline Salt

Number of Solvents

**Sol1**

Average Residence Time of Solvent Around Cation

Average Residence Time of Solvent Around Anion

Cation Reference Solvation Number

Anion Reference Solvation Number

Index for Solvent Solvation Configuration Around Cation

Index for Solvent Solvation Configuration Around Anion

Parameter for Solvent Solvation Configuration Around Cation

Parameter for Solvent Solvation Configuration Around Anion

Save
Close

**Figure 172. ACCC Salt Definition for LiPF6\_w\_EC**

**Edit ACCC Salt Class**

Salt Class Name

Salt Identifier

Regular Salt
Ionic Liquid

Diameter of Cation from Crystalline Basis

Diameter of Anion from Crystalline Basis [Å]

Equivalent Diameter of Anion Accounting for Electrostatic Charge Distribution of Anion

Number of Charge Regions for Anion

Unit Charge of Cation

Unit Charge of Anion

Molecular Weight of Salt

Molecular Weight of Cation

Density of Pure Crystalline Salt

Relative Permittivity of Pure Crystalline Salt

Number of Solvents

**Sol1**
**Sol2**

Average Residence Time of Solvent Around Cation

Average Residence Time of Solvent Around Anion

Cation Reference Solvation Number

Anion Reference Solvation Number

Index for Solvent Solvation Configuration Around Cation

Index for Solvent Solvation Configuration Around Anion

Parameter for Solvent Solvation Configuration Around Cation

Parameter for Solvent Solvation Configuration Around Anion

Save
Close

## Advanced Electrolyte Model (AEM)

Sol1 Sol2

1.01 ns ⓘ	0.45 ns ⓘ	2. ⓘ	2. ⓘ
Average Residence Time of Solvent Around Cation	Average Residence Time of Solvent Around Anion	Cation Reference Solvation Number	Anion Reference Solvation Number
8 ⓘ	2 ⓘ	1.3 ⓘ	1.6 ⓘ
Index for Solvent Solvation Configuration Around Cation	Index for Solvent Solvation Configuration Around Anion	Parameter for Solvent Solvation Configuration Around Cation	Parameter for Solvent Solvation Configuration Around Anion

[Save](#) [Close](#)

**Figure 173. ACCC Salt Definition for LiBOB\_w\_EC\_EM.**

Edit ACCC Salt Class

LiPF6_w_EM		Salt Class Name	
LiPF6		Salt Identifier	
<input checked="" type="radio"/> Regular Salt		<input type="radio"/> Ionic Liquid	
Salt Type			
1.36 Å ⓘ	4.9 Å ⓘ	4.9 Å ⓘ	1. ⓘ
Diameter of Cation from Crystalline Basis	Diameter of Anion from Crystalline Basis [Å]	Equivalent Diameter of Anion Accounting for Electrostatic Charge Distribution of Anion	Number of Charge Regions for Anion
1. ⓘ	-1. ⓘ	151.90 g/mole ⓘ	6.941 g/mole ⓘ
Unit Charge of Cation	Unit Charge of Anion	Molecular Weight of Salt	Molecular Weight of Cation
2.6 g/cm³ ⓘ	19. ⓘ		
Density of Pure Crystalline Salt	Relative Permittivity of Pure Crystalline Salt		
1 ⓘ			
Number of Solvents			

Sol1

1.01 ns ⓘ	0.45 ns ⓘ	2. ⓘ	2. ⓘ
Average Residence Time of Solvent Around Cation	Average Residence Time of Solvent Around Anion	Cation Reference Solvation Number	Anion Reference Solvation Number
8 ⓘ	2 ⓘ	1.3 ⓘ	1.6 ⓘ
Index for Solvent Solvation Configuration Around Cation	Index for Solvent Solvation Configuration Around Anion	Parameter for Solvent Solvation Configuration Around Cation	Parameter for Solvent Solvation Configuration Around Anion

[Save](#) [Close](#)

**Figure 174. ACCC Salt Definition for LiBOB\_w\_EC\_EM.**

## Advanced Electrolyte Model (AEM)

Edit ACCC Salt Class

PYR13-FSI\_w\_EC\_EMCSalt Class Name

PYR13-FSISalt Identifier

Regular Salt Ionic Liquid  
Salt Type

1.776 Å ⓘ Diameter of Cation from Crystalline Basis	5.66 Å ⓘ Diameter of Anion from Crystalline Basis [Å]	4.811 Å ⓘ Equivalent Diameter of Anion Accounting for Electrostatic Charge Distribution of Anion	1. ⓘ Number of Charge Regions for Anion
1. ⓘ Unit Charge of Cation	-1. ⓘ Unit Charge of Anion	308.37 g/mole ⓘ Molecular Weight of Salt	128.37 g/mole ⓘ Molecular Weight of Cation
1.33 g/cm³ ⓘ Density of Pure Crystalline Salt	22. ⓘ Relative Permittivity of Pure Crystalline Salt	1.0 ⓘ RTIL Factor to Express Cation Diameter	1.0 ⓘ Number of Charge Regions for Cation
2 ⓘ Number of Solvents			
Sol1 Sol2			
1.15 ns ⓘ Average Residence Time of Solvent Around Cation	0.32 ns ⓘ Average Residence Time of Solvent Around Anion	5. ⓘ Cation Reference Solvation Number	1.5 ⓘ Anion Reference Solvation Number
10 ⓘ Index for Solvent Solvation Configuration Around Cation	2 ⓘ Index for Solvent Solvation Configuration Around Anion	1.28 ⓘ Parameter for Solvent Solvation Configuration Around Cation	1.22 ⓘ Parameter for Solvent Solvation Configuration Around Anion

Save Close

**Figure 175. ACCC Salt Definition for LiBOB\_w\_EC\_EMCS.**

## 7.4 ACCC Validation Examples

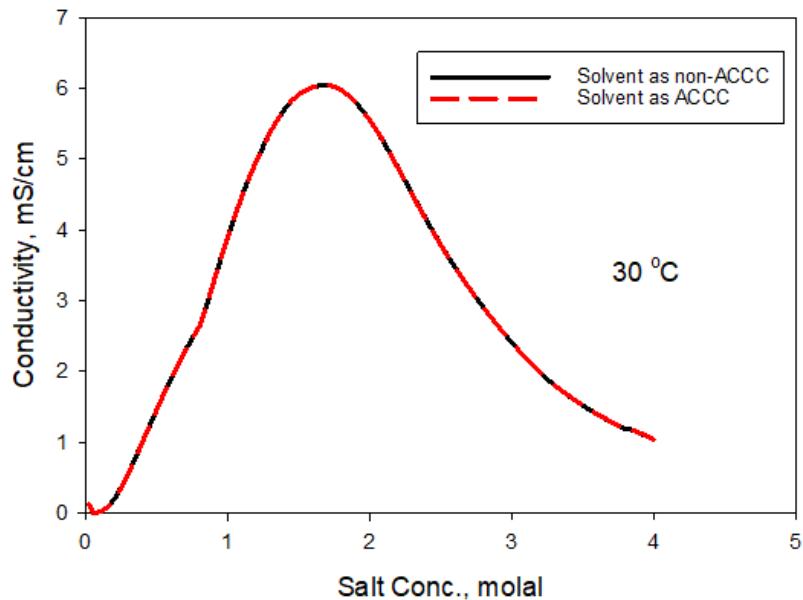


Figure 176. EMC+LiPF<sub>6</sub> at 30°

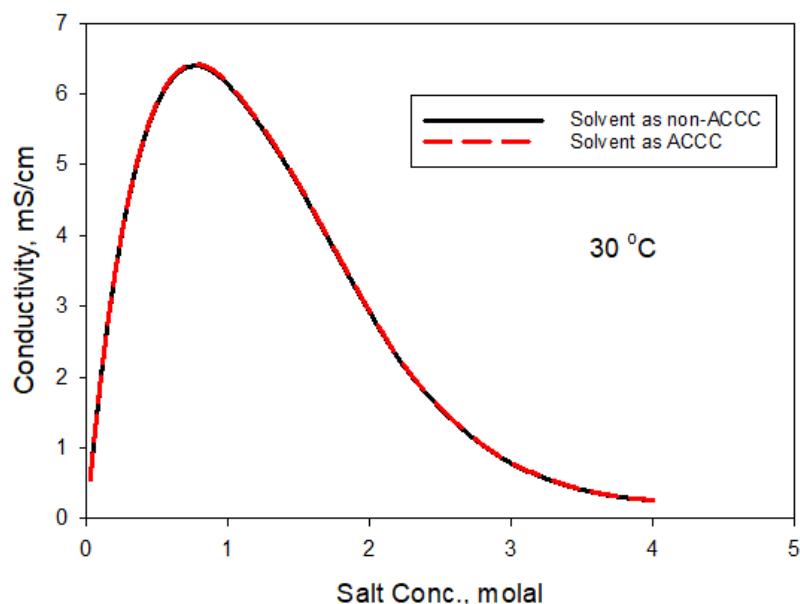
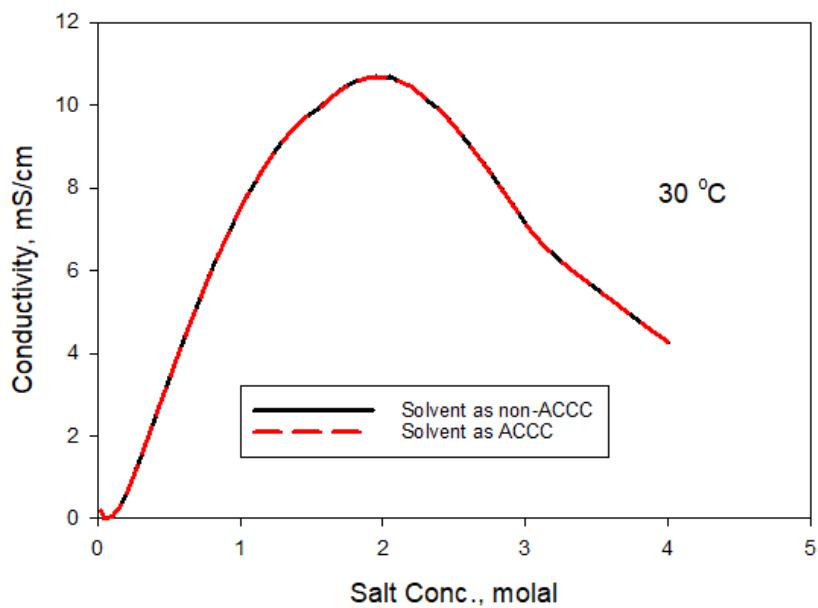
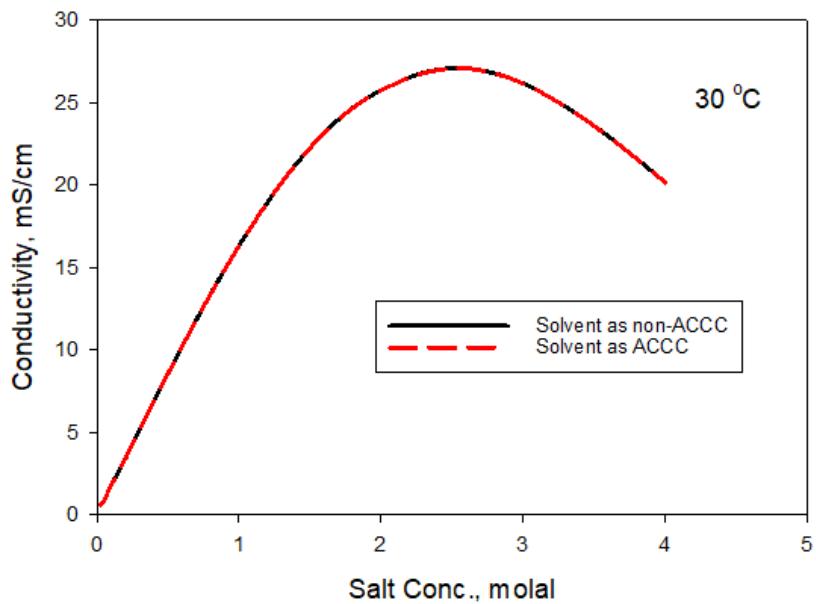


Figure 177. PC+LiPF<sub>6</sub> at 30°

### Advanced Electrolyte Model (AEM)



**Figure 178. DMC+LiPF<sub>6</sub> at 30°**



**Figure 179. MA+LiPF<sub>6</sub> at 30°**

### Advanced Electrolyte Model (AEM)

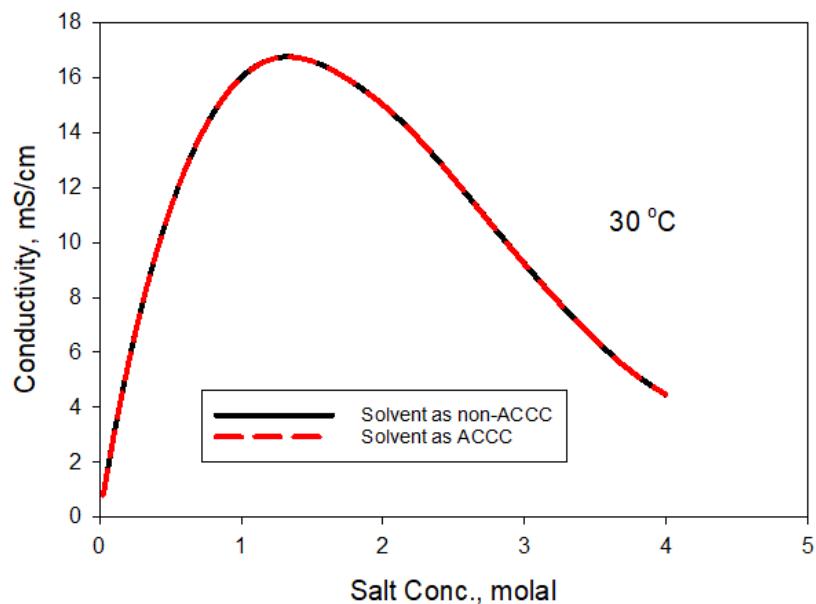


Figure 180. BN+LiPF<sub>6</sub> at 30°

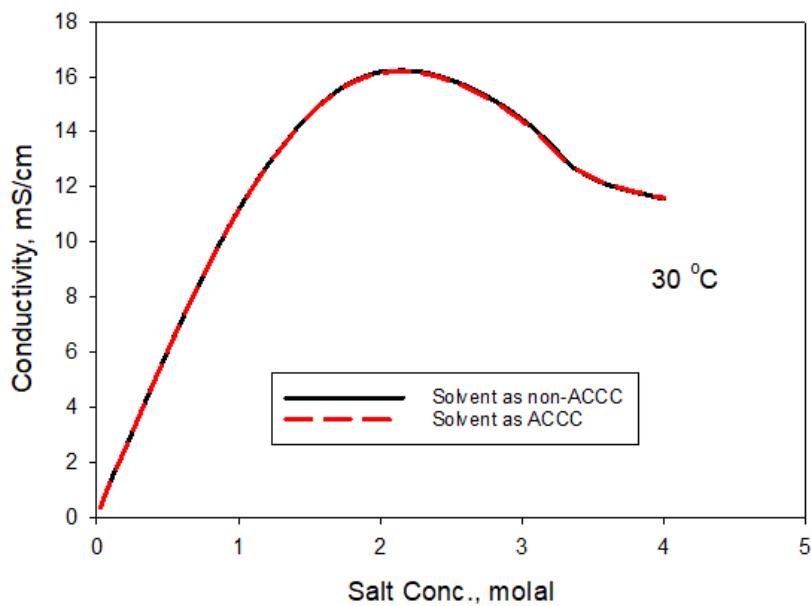


Figure 181. DME+LiPF<sub>6</sub> at 30°

### Advanced Electrolyte Model (AEM)

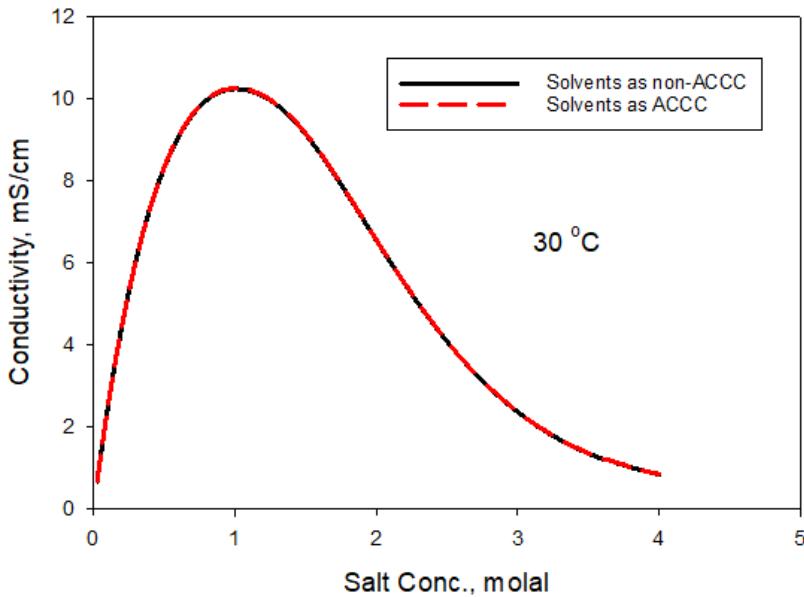


Figure 182. PC-EMC (4:6 by mass)+LiPF<sub>6</sub> at 30°

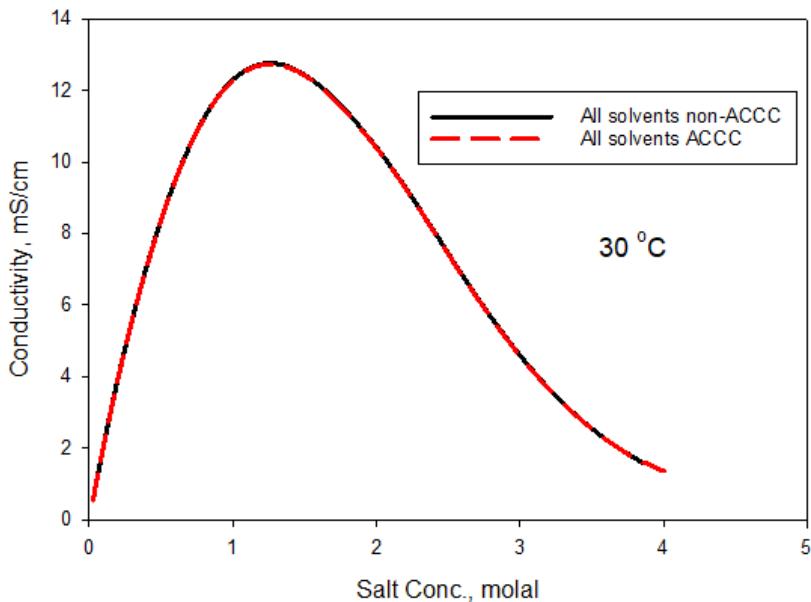
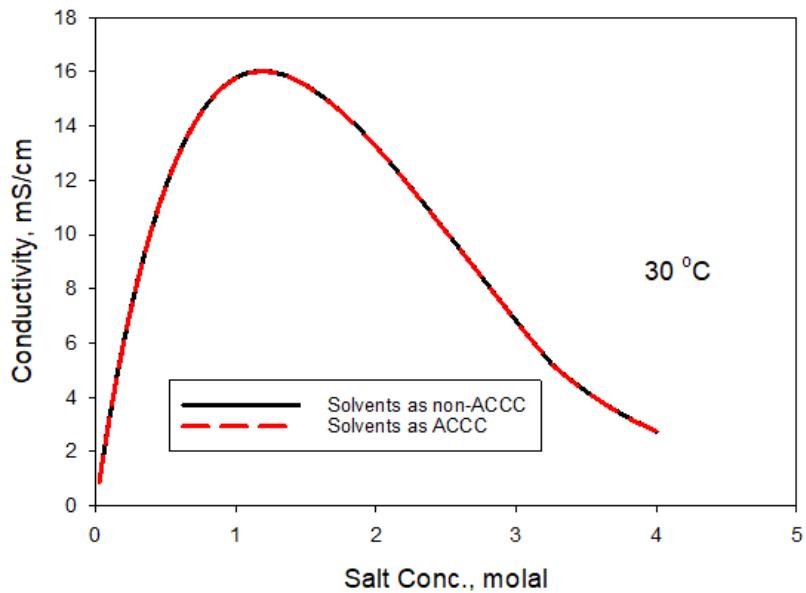
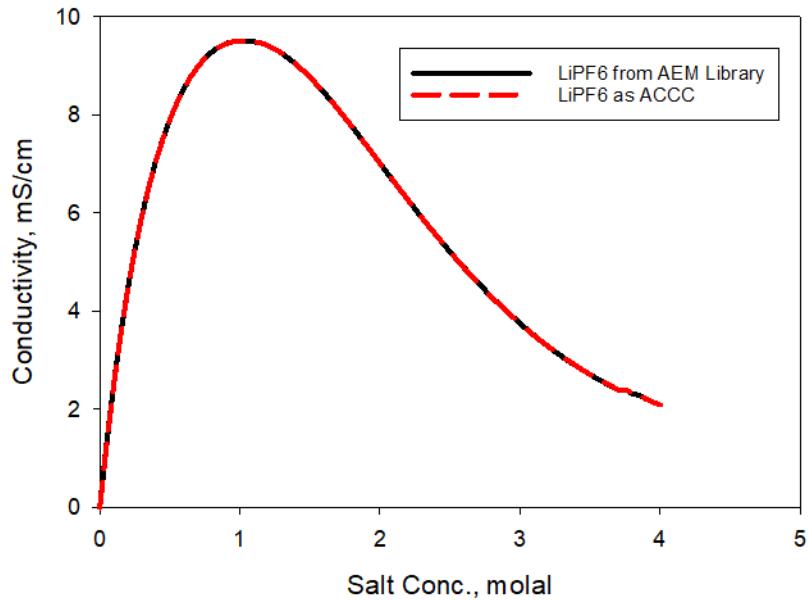


Figure 183. EC-DMC-nPA (2:5:3 by mass)+LiPF<sub>6</sub> at 30°

### Advanced Electrolyte Model (AEM)

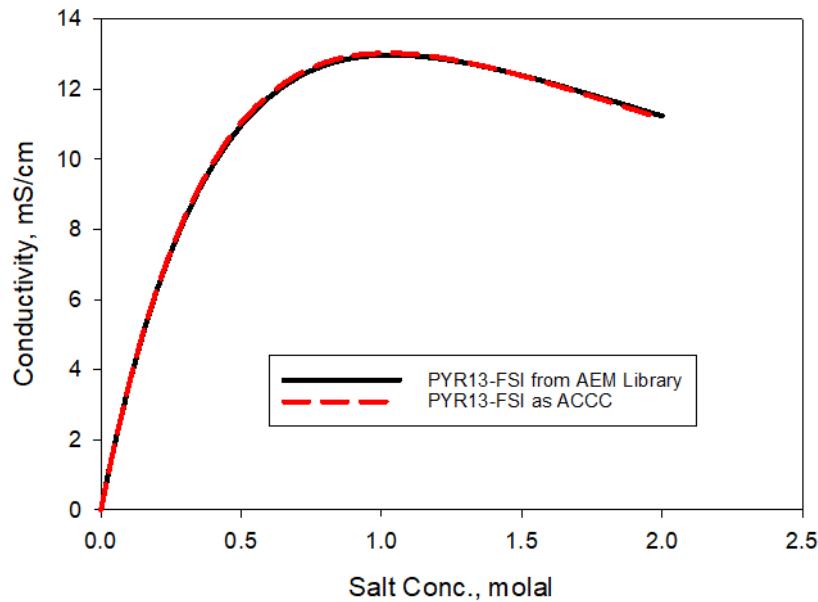


**Figure 184. PC-EC-EMC-MA-BN (1:1:1:1:1 by mass)+LiPF<sub>6</sub> at 30°**

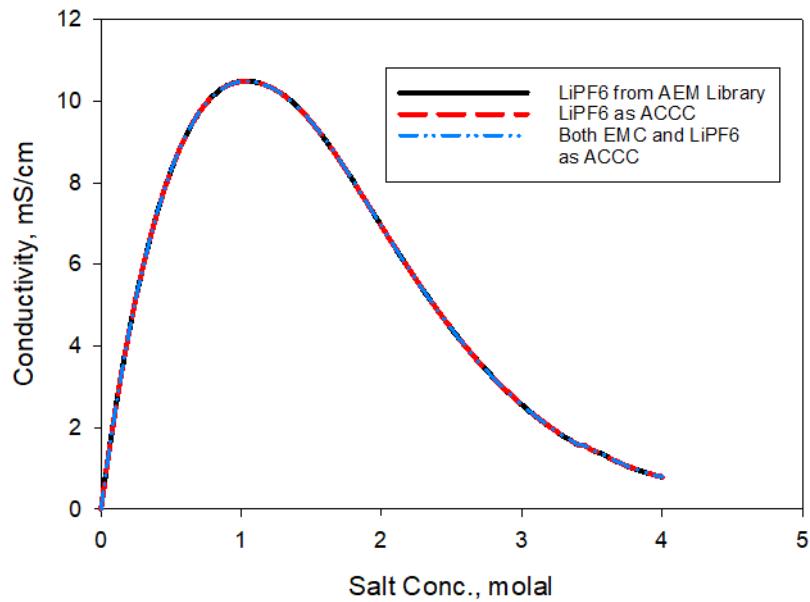


**Figure 185. EC-EMC (3:7 by mass)+(0.5LiPF<sub>6</sub> + 0.5LiFSI)**

### Advanced Electrolyte Model (AEM)

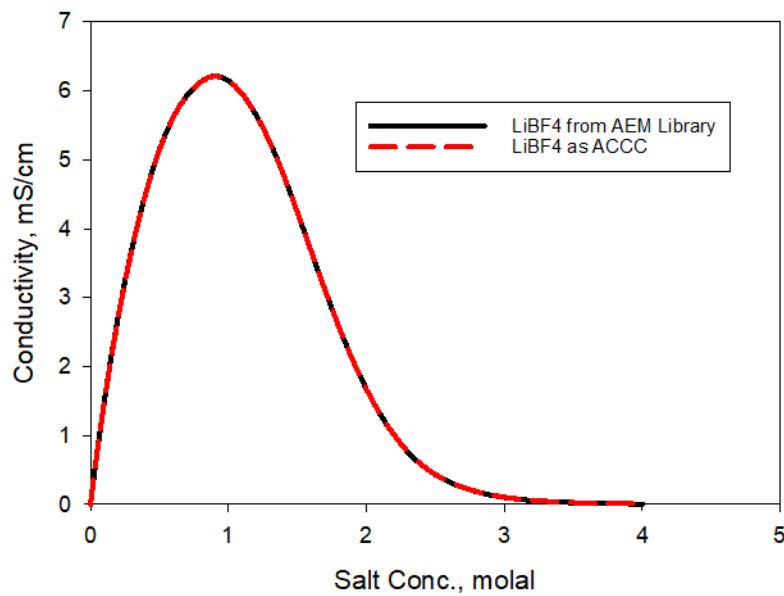


**Figure 186. EC-EMC (3:7 by mass)+ PYR13-FSI**



**Figure 187. EC-EMC (3:7 by mass)+LiPF<sub>6</sub>**

### Advanced Electrolyte Model (AEM)



**Figure 188. EC-EMC (2:8 by mass)+LiBF<sub>4</sub>**

## **7.5 List of Relevant Publications**

The following list provides a partial list of relevant AEM publications.

- A Critical Evaluation of the Advanced Electrolyte Model
- A Study of the Transport Properties of Ethylene Carbonate-Free Li Electrolytes
- Nonaqueous Liquid Electrolytes for Lithium-Based Rechargeable Batteries
- A Study of the Physical Properties of Li-ion Battery Electrolytes Containing Esters
- An automated system for performing continuous viscosity *versus* temperature measurements of fluids using an Ostwald viscometer
- Synergistic Effect of LiPF<sub>6</sub> and LiBF<sub>4</sub> as Electrolyte Salts in Lithium-Ion Cells
- Prediction of Electrolyte Conductivity: Results from a Generalized Molecular Model Based on Ion Solvation and a Chemical Physics Framework
- Macro-homogenous Modeling of Commercial, Primary Li/MnO<sub>2</sub> Coin Cells
- Prediction of electrolyte viscosity for aqueous and non-aqueous systems: Results from a molecular model based on ion solvation and a chemical physics framework
- Low-Temperature Performance Limitations of Lithium-ion Batteries
- Novel Method for Evaluation and Prediction of Capacity Loss Metrics in Li-Ion Electrochemical Cells
- An Experimental and Modeling Study of Sodium-ion Battery Electrolytes
- Methodologies for Design, Characterization and Testing of Electrolytes that Enable Extreme Fast Charging of Lithium-ion Cells

Additional publications may also be highlighted on the Ridgetop and INL product pages in accordance with the rules and regulations of publishing journals, conferences, and other related organizations.

- <https://www.ridgetopgroup.com/about-us/ridgetop-affiliates/advanced-electrolyte-model-aem-developed-by-idaho-national-laboratory/>
- <https://labpartnering.org/technologies/b361487d-0e61-4fe1-9ba8-4d004a8dc4a2>

## **Advanced Electrolyte Model (AEM)**

## 7.6 Table of Figures

Figure 1. AEM Framework .....	2
Figure 2. 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).....	4
Figure 3. AEM Overview.....	5
Figure 4. AEM installation folder saved in This PC > Downloads.....	7
Figure 5. The folder is located at This PC\Downloads\[AEM Download Path].....	8
Figure 6. AEM installation wizard initializing.....	8
Figure 7. View of the installation wizard for the AEM installation directory. Click Next> to continue.....	9
Figure 8. View of the AEM GUI when it starts after a fresh installation.....	9
Figure 9. AEM GUI pop-up indicating successful software license activation.....	10
Figure 10. Selecting Default Program Directory during AEM Installation Process.....	11
Figure 11. Verifying AEM Software Version. ....	11
Figure 12. Tab 1 – AEM Input. ....	12
Figure 13. Solvent Composition Mode Toggle Switches in the AEM Input tab. ....	13
Figure 14. SELECT SOLVENTS section for the SINGLE FIXED COMPOSITION OF SOLVENTS option of the AEM Input tab.....	14
Figure 15. Drop-down List Button to select solvents for the SINGLE FIXED COMPOSITION OF SOLVENTS option of the AEM Input tab.....	14
Figure 16. Percentage of Solvent input depending on Volume/Mass for each solvent for the SINGLE FIXED COMPOSITION OF SOLVENTS option of the AEM Input tab.....	15
Figure 17. SELECT SOLVENTS section for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab.....	16
Figure 18. Drop-down List Button to select solvents for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab. ....	16
Figure 19. SELECT SOLVENTS section for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab in the case of less than or equal to two (2) total solvents. ....	17
Figure 20. SELECT SOLVENTS section for the LARGER MATRIX OF SOLVENT COMPOSITION FOR OPTIMIZATION OF ELECTROLYTE FORMULATION option of the AEM Input tab in the case of greater than two (2) total solvents.....	17
Figure 21. Solvent list in AEM Version 2.24.1 with recent additions including 55-TEP, 56-BTFE, 57-TTE, 58-E2FA, 59-DMP, 60-DMS, 61-IVN, and 62-IBN. Note that only select solvents are available in the AEM Trial Version.....	18
Figure 22. SELECT SALTS section of the AEM Input tab.....	19

## Advanced Electrolyte Model (AEM)

Figure 23. Drop-down List Button to select salts for the SELECT SALTS section of the AEM Input tab.....	20
Figure 24. SELECT SALTS section of the AEM Input tab for 1 salt.....	20
Figure 25. SELECT SALTS section of the AEM Input tab for 2 salts.....	21
Figure 26. Single vs Range Composition Proportion Mode for the SELECT SALTS section of the AEM Input tab for 2 salts. ....	22
Figure 27. Salt list in AEM Version 2.24.1 with recent additions including 38-LiDFBOP. Note that only select Salts are available in the AEM Trial Version. ....	23
Figure 28. TEMPERATURE SETTINGS section of the AEM Input tab.....	24
Figure 29. TEMPERATURE SETTINGS section of the AEM Input tab.....	24
Figure 30. ELECTROLYTE INGRESS INTO PORES section of the AEM Input tab. ....	25
Figure 31. SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP) section of the AEM Input tab with a check box to perform SCAEP Calculations not checked (default). ....	25
Figure 32. SURFACE-CHARGE ATTENUATED ELECTROLYTE PERMITTIVITY (SCAEP) section of the AEM Input tab with a check box to perform SCAEP Calculations checked.....	26
Figure 33. DOUBLE LAYER (DL) section of the AEM Input tab with check box to perform DL Calculations not checked (default). ....	26
Figure 34. DOUBLE LAYER (DL) section of the AEM Input tab with a check box to perform DL Calculations checked. ....	27
Figure 35. AEM RUN IDENTIFIER section of the AEM Input tab. ....	27
Figure 36. RUN AEM Button of the AEM Input tab.....	28
Figure 37. Prompt showing AEM running after the RUN AEM Button of the AEM Input tab is clicked.....	28
Figure 38. Prompt showing AEM Run Complete. ....	28
Figure 39. AEM Run Error.....	29
Figure 40. ERROR_OCCURED.txt located at C:\Users\user-name\Documents\AEM\DATA\[Simulation Folder Name].....	29
Figure 41. ERROR_OCCURED.txt as viewed in a Text Editor.....	30
Figure 42. AEM ACCC Overview Diagram.....	32
Figure 43. AEM ACCC Solvent Class GUI View.....	33
Figure 44. Note for time-average ion solvation.....	36
Figure 45. ACCC Solvent Definition for Butryonitrile (BN). ....	37
Figure 46. AEM ACCC Salt Class GUI View. ....	39
Figure 47. ACCC Salt Definition for LiBF4_w_EC_EM.....	42
Figure 48. EC+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	43
Figure 49. PC-EA (3:7 by mass) + LiBOB.....	43
Figure 50. Tab 1 – AEM Output with REPORT TEXT section.....	44
Figure 51. Tab 1 – AEM Output with REPORT DATA VISUALIZATION section.....	45

Figure 52. AEM RUNS section of the AEM Output tab.....	45
Figure 53. AEM REPORTS section of the AEM Output tab.....	47
Figure 54. Data Display section of the AEM Output tab.....	47
Figure 55. REPORT TEXT section of the AEM Output tab – Viewing the Report01 – Report20 Output Report files. ....	48
Figure 56. REPORT TEXT section of the AEM Output tab – Viewing the settings .json file. ....	48
Figure 57. REPORT TEXT section of the AEM Output tab – Viewing the verbose .txt file. ....	49
Figure 58. REPORT DATA VISUALIZATION section of the AEM Output tab – 3 select drop down options..	49
Figure 59. REPORT DATA VISUALIZATION section of the AEM Output tab. ....	50
Figure 60. Single Paramter Export Feature.....	51
Figure 61. Layout for the csv exported for a single parameter.....	51
Figure 62. EXPORT ALL Feature .....	52
Figure 63. Layout for the csv exported for EXPORT ALL feature .....	53
Figure 64. Icon for GUI Import Button. ....	53
Figure 65. Icon for GUI Reset Inputs Button. ....	54
Figure 66. Icon and pop-up message for GUI Information Button. ....	54
Figure 67. Icon and pop-up message for GUI Help Button.....	54
Figure 68. Icon and visual aid for Expanded Format (Top) and Compact Format (Bottom). ....	55
Figure 69. Icon and pop-up message when changing the default program directory. ....	56
Figure 70. Icon and visual aid for GUI in Light Mode (Top) and Dark Mode (Bottom). ....	57
Figure 71. Icon and pop-up message for the Exit Button. ....	58
Figure 72. Importing Example 1 Input Condition using the settings-Example 1.json file. ....	60
Figure 73. Example 1 – AEM Input tab.....	61
Figure 74. Example 1 – AEM Output tab – REPORT TEXT section to view Report01-Report20. ....	62
Figure 75. Example 1 – Diffusivity/Diffusion Coefficient (cm <sup>2</sup> /s) v/s Molal Salt Conc. (m2). ....	62
Figure 76. Example 1 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).....	63
Figure 77. Example 1 – Viscosity (cP) v/s Molal Salt Conc. (m2).....	63
Figure 78. Example 1 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. (m2). ....	64
Figure 79. Example 1 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. (m2). ....	64
Figure 80. Importing Example 2 Input Condition using the settings-Example 2.json file. ....	66
Figure 81. Example 2 – AEM Input tab.....	67
Figure 82. Example 2 – AEM Output tab – REPORT TEXT section to view Report01-Report20. ....	68
Figure 83. Example 2 – Diffusivity/Diffusion Coefficient (cm <sup>2</sup> /s) v/s Molal Salt Conc. (m2). ....	69
Figure 84. Example 2 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).....	69

Figure 85. Example 2 – Viscosity (cP) v/s Molal Salt Conc. (m2).....	70
Figure 86. Example 2 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. (m2). ....	70
Figure 87. Example 2 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. (m2).....	71
Figure 88. Importing Example 3 Input Condition using the settings-Example 3.json file. ....	73
Figure 89. Example 3 – AEM Input tab.....	74
Figure 90. Example 3 – AEM Output tab – REPORT TEXT section to view Report01-Report20. ....	75
Figure 91. Example 3 – Diffusivity/Diffusion Coefficient (cm <sup>2</sup> /s) v/s Molal Salt Conc. (m2). ....	75
Figure 92. Example 3 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).....	76
Figure 93. Example 3 – Viscosity (cP) v/s Molal Salt Conc. (m2).....	76
Figure 94. Example 3 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. (m2). ....	77
Figure 95. Example 3 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. (m2). ....	77
Figure 96. Importing Example 4 Input Condition using the settings-Example 5.json file. ....	79
Figure 97. Example 4 – AEM Input tab.....	80
Figure 98. Example 4 – AEM Output tab – REPORT TEXT section to view Report01-Report20. ....	81
Figure 99. Example 4 – Diffusivity/Diffusion Coefficient (cm <sup>2</sup> /s) v/s Molal Salt Conc. (m2). ....	81
Figure 100. Example 4 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).....	82
Figure 101. Example 4 – Viscosity (cP) v/s Molal Salt Conc. (m2). ....	82
Figure 102. Example 4 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. (m2). ....	83
Figure 103. Example 4 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. (m2).....	83
Figure 104. Importing Example 5 Input Condition using the settings-Example 5.json file.....	85
Figure 105. Example 5 – AEM Input tab .....	86
Figure 106. Example 5 – AEM Output tab – REPORT TEXT section to view Report01-Report20.....	87
Figure 107. Importing Example 6 Input Condition using the settings-Example 6.json file.....	88
Figure 108. Example 6 – AEM Input tab .....	89
Figure 109. Example 6 – AEM Output tab – REPORT TEXT section to view Report01-Report20.....	90
Figure 110. Example 6 – Diffusivity/Diffusion Coefficient (cm <sup>2</sup> /s) v/s Molal Salt Conc. (m2). ....	91
Figure 111. Example 6 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).....	91
Figure 112. Example 6 – Viscosity (cP) v/s Molal Salt Conc. (m2). ....	92
Figure 113. Example 6 – Cation Transference No. ( $t_+(a)$ ) v/s Molal Salt Conc. (m2). ....	92
Figure 114. Example 6 – Cation Transference No. ( $t_+(b)$ ) v/s Molal Salt Conc. (m2). ....	93
Figure 115. Importing Example 7 Input Condition using the settings-Example 7.json file.....	95
Figure 116. Example 7 – AEM Input tab .....	96
Figure 117. Example 7 - AEM Output tab – REPORT TEXT section to view Report01-Report20.....	97

Figure 118. Example 7 – Diffusivity/Diffusion Coefficient (cm <sup>2</sup> /s) v/s Molal Salt Conc. (m2).....	97
Figure 119. Example 7 – Specific Conductivity (mS/cm) v/s Molal Salt Conc. (m2).....	98
Figure 120. Example 7 – Viscosity (cP) v/s Molal Salt Conc. (m2) .....	98
Figure 121. Example 7 – Cation Transference No. (t+(a)) v/s Molal Salt Conc. (m2).....	99
Figure 122. Example 7 – Cation Transference No. (t+(b)) v/s Molal Salt Conc. (m2) .....	99
Figure 123. AEM Fortran Version 2.24.2 Program Flow – single fixed composition of solvents is chosen in A.1.....	100
Figure 124. AEM Fortran Version 2.24.2 Program Flow – larger matrix of solvent composition is chosen in A.1.....	101
Figure 125. aem-2242m-d-accc CLI Executable in ...\\AEM\\CLI\\.....	102
Figure 126. Welcome Message prompt when AEM is first run.....	102
Figure 127. Section A.1 from AEM Fortran Version 2.24.2.....	103
Figure 128. Prompt to Input 1 for Section A.1 from AEM Fortran Version 2.24.2.....	103
Figure 129. Section A.2F from AEM Fortran Version 2.24.2.....	104
Figure 130. Section A.3 (1) from AEM Fortran Version 2.24.2.....	104
Figure 131. Selecting solvents in CLI Example 1.....	105
Figure 132. Section A.3 (2) from AEM Fortran Version 2.24.2.....	105
Figure 133. Section A.4 from AEM Fortran Version 2.24.2.....	105
Figure 134. Section A.5 from AEM Fortran Version 2.24.2.....	106
Figure 135. Section A.8 from AEM Fortran Version 2.24.2.....	107
Figure 136. Section B.1 from AEM Fortran Version 2.24.2 .....	107
Figure 137. Section B.2 from AEM Fortran Version 2.24.2 .....	108
Figure 138. Section B.3 from AEM Fortran Version 2.24.2 .....	108
Figure 139. Section B.4 from AEM Fortran Version 2.24.2 .....	109
Figure 140. Section C from AEM Fortran Version 2.24.2.....	109
Figure 141. Section D from AEM Fortran Version 2.24.2 .....	110
Figure 142. Section E from AEM Fortran Version 2.24.2 .....	111
Figure 143. The different output files generated by AEM are highlighted inside the blue box. ....	112
Figure 144. The modular AEM API Architecture.....	113
Figure 145. Selecting the option python.exe checkbox during the Python installation. ....	115
Figure 146. The folder structure for the default AEM directory.....	116
Figure 147. ACCC compositions within the ACCC\\ directory.....	116
Figure 148. Opening default AEM user directory in VS Code.....	117
Figure 149. View of VS Code Window after cloning AEM-API from Github.....	118

## Advanced Electrolyte Model (AEM)

Figure 150. A visual of the command line while installing dependencies.....	119
Figure 151. A visual from VS Code when the when AEM_API_wACCC_allACCCcomp.py script is run from the Terminal.....	120
Figure 152. View of data output directory from AEM simulation using Python API.....	120
Figure 153. Cation Transference No. [t+(a) & t+(b)] (left) and Mean Viscosity (right) as a function of Molal (m) and Molar (c) Salt Concentrations.....	124
Figure 154. Density (g/mL) (left) and Combined Conductivity (right) as a function of Molal (m) and Molar (c) Salt Concentrations.....	124
Figure 155. ACCC Solvent Definition for DMC.....	139
Figure 156. ACCC Solvent Definition for DME.....	140
Figure 157. ACCC Solvent Definition for EC.....	141
Figure 158. ACCC Solvent Definition for EC-DMC-NPA.....	142
Figure 159. ACCC Solvent Definition for EC-EMC.....	143
Figure 160. ACCC Solvent Definition for EC-PC-EMC-MA-BN.....	144
Figure 161. ACCC Solvent Definition for EMC.....	145
Figure 162. ACCC Solvent Definition for EP.....	146
Figure 163. ACCC Solvent Definition for EP-BN.....	147
Figure 164. ACCC Solvent Definition for MA.....	148
Figure 165. ACCC Solvent Definition for NPA.....	149
Figure 166. ACCC Solvent Definition for PC .....	150
Figure 167. ACCC Solvent Definition for PC-EC-EMC-MA-BN.....	151
Figure 168. ACCC Solvent Definition for PC-EMC.....	152
Figure 169. ACCC Solvent Definition for PN.....	153
<b>Figure 170. ACCC Solvent Definition for VEC.</b> .....	154
Figure 171. ACCC Salt Definition for LiBOB_w_PC_EA .....	155
Figure 172. ACCC Salt Definition for LiPF <sub>6</sub> _w_EC .....	156
Figure 173. ACCC Salt Definition for LiBOB_w_EC_EMC.....	157
Figure 174. ACCC Salt Definition for LiBOB_w_EC_EMC.....	157
Figure 175. ACCC Salt Definition for LiBOB_w_EC_EMC.....	158
Figure 176. EMC+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	159
Figure 177. PC+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	159
Figure 178. DMC+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	160
Figure 179. MA+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	160
Figure 180. BN+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	161

## **Advanced Electrolyte Model (AEM)**

Figure 181. DME+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	161
Figure 182. PC-EMC (4:6 by mass)+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	162
Figure 183. EC-DMC-nPA (2:5:3 by mass)+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	162
Figure 184. PC-EC-EMC-MA-BN (1:1:1:1:1 by mass)+LiPF <sub>6</sub> at 30 <sup>0</sup> .....	163
Figure 185. EC-EMC (3:7 by mass)+(0.5LiPF <sub>6</sub> +0.5LiFSI).....	163
Figure 186. EC-EMC (3:7 by mass)+ PYR13-FSI .....	164
Figure 187. EC-EMC (3:7 by mass)+LiPF <sub>6</sub> .....	164
Figure 188. EC-EMC (2:8 by mass)+LiBF <sub>4</sub> .....	165

**Software User Guide for the  
Advanced Electrolyte Model (AEM)  
Developed by Idaho National  
Laboratory**

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