RESEARCH BRIEF
Start Date: Oct 1 2020 | Duration: 24 months

NAWI National Alliance for Water Innovation

# Open-Source Modeling & Optimization Library for Water Treatment Processes

**George Bollas** | University of Connecticut
george.bollas@uconn.edu

## Challenge

Understanding the properties of brines is critical in the design, control, and optimization of brine concentrator treatment systems. Typically, thermodynamic models are used to derive the properties of pure substances and their mixtures; however, these models are largely incomplete because salt behavior in highly concentrated brines is poorly understood and existing models cannot be extrapolated with a high degree of accuracy. Understanding of the thermodynamic and kinetic phenomena in concentrated multi-electrolyte, mixed-solvent solutions, such as those in brines, is a hundred-year old challenge originating in the pioneering work of Peter Debye that awarded him the Nobel Prize in 1936. These old theories and existing models have significant limitations when applied to solutions as concentrated and complex as brines from water treatment facilities. Moreover, available models have not been developed for modern optimization platforms and cannot support process intensification and digital twin applications.

## Research Approach

The project aims to develop a new, more accurate theory for the properties of high salinity brines. This improved understanding will be used to develop a new, open-source modeling library and framework, which will in turn inform and refine existing NAWI tools, such as ProteusLib and Water-TAP3. The project will generate thermodynamic, thermal, transport, and speciation data for concentrated brines. The team will coordinate modeling and experimental efforts for the design of experiments for brines characterization, the discovery of principal model dependencies, and the tuning of models to accurately predict the properties of brines. Work is also planned for the deployment and validation of these models in ProteusLib and the certification of the models to meet modern software standards that allow these models to be used for optimization, control, and monitoring of water treatment processes.

### RESEARCH PARTNERS

Modelon, Inc.: Chen Chen, Hubertus Tummescheit; Sandia National Laboratories: Jordan Jalving; University of Connecticut: Edward Wazer, George Bollas, Jeffrey McCutcheon, Matthew Stuber, Maur Ostwal.

## Impact

With a unique combination of expertise in electrolyte thermodynamics, process modeling, optimization, and water separation processes, the UConn/Sandia/Modelon team is uniquely positioned to overcome the limitations of today's state-of-the-art in the simulation, synthesis, and design of water treatment processes and contribute to the vision of the U.S. DOE for a sustainable future in the food-water-energy nexus. This project is expected to disrupt the existing practices of designing water treatment facilities by providing an open-source software that is open to all NAWI users and can be integrated with parallel efforts such as Water-TAP3. Enabling the accurate simulation of concentrated brine solutions and treatment systems will allow for greater utilization and reuse of non-traditional water sources, by allowing out-of-the-box studies and re-design optimization of existing systems.

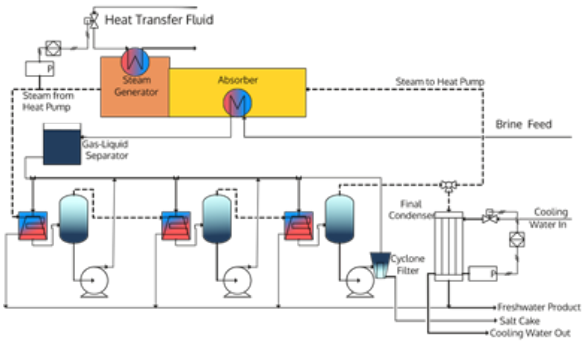


**Figure 1.** Architecture of a heat integrated multi-effect brine concentrator to be designed and optimized.

### REFERENCES

1. Bollas GM et al. Refined Electrolyte-NRTL Model : Activity Coefficient Expressions for Application to Multi-Electrolyte Systems. AIChE J. 2008;54(6):1608-1624.
2. Bollas GM et al. Bilevel optimization formulation for parameter estimation in vapor-liquid(-liquid) phase equilibrium problems. Chem Eng Sci. 2009;64:1768-1783.
3. Mitsos A,et al. Bilevel optimization formulation for parameter estimation in liquid–liquid phase equilibrium problems. Chem Eng Sci. 2009;64(3):548-559.
4. Stuber MD et al. Pilot demonstration of concentrated solar-powered desalination of subsurface agricultural drainage water and other brackish groundwater sources. Desalination. 2015;355:186-196.

This work was supported by the National Alliance for Water Innovation (NAWI), funded by the U.S. Department of Energy, Energy Efficiency and Renewable Energy Office, Advanced Manufacturing Office.

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY