NAWI
National Alliance
for Water Innovation

ProteusLib: Integrated Computational Capability for Optimizing Advanced Water Treatment Systems

Tim Bartholomew | National Energy Technology Laboratory (NETL)

Timothy.Bartholomew@netl.doe.gov

Challenge

At the system level, there is no comprehensive commercial process simulation software available to model and optimize full water treatment trains. Thus, it is difficult to compare existing products and materials from different manufacturers or consider new and novel technologies in the context of a full treatment train.

Research Approach

We are addressing this critical gap by developing ProteusLib, a modeling and simulation capability for the design and optimization of water treatment systems. ProteusLib is a modular water treatment model library that can be used on the IDAES Platform, an advanced process systems engineering tool developed by the U.S. Department of Energy. ProteusLib will enable users to perform detailed technoeconomic assessments of treatment trains made up of the supported models, while leveraging the benefits of an open source, extensible, and equation oriented computational capability.

Impact

Within its first year of work, ProteusLib developers created models representing a full RO treatment train including pre- and post-treatment. Besides demonstrating the advanced optimization capabilities for the conventional seawater RO desalination, the flexibility of the platform was demonstrated through technoeconomic assessments of early-stage treatment technologies including high pressure reverse osmosis and low salt rejection reverse osmosis.

ProteusLib capabilities are being combined with WaterTAP3, another NAWI modeling effort, to form a merged tool called WaterTAP.
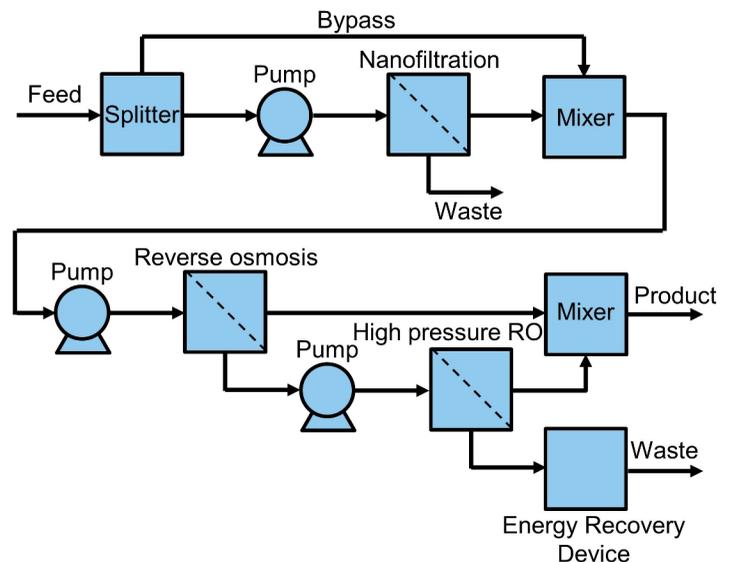
Figure 1. Example ProteusLib flowsheet of a water treatment train including nanofiltration pretreatment and conventional and high pressure reverse osmosis desalination that can be cost optimized subject to constraints on gypsum scaling.

RESEARCH PARTNERS

Lawrence Berkeley National Laboratory (LBNL): Daniel Gunter, Jangho Park, Keith Beattie, Ludovico Bianchi, Oluwamayowa Amusat; National Energy Technology Laboratory (NETL): Adam Atia, Andres Calderon-Vergara, Andrew Lee, Anthony Burgard, David Miller, Markus Drouven, Tim Bartholomew; National Renewable Energy Laboratory (NREL): Bernard Knueven, Ethan Young, Jeffrey Allen; Oak Ridge National Laboratory (ORNL): Austin Ladshaw, Srikanth Allu.

REFERENCES

1. For an overview presentation on Proteuslib, click here.
2. For more information on IDAES, visit this link.

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