

Desalination and brine treatment systems integrated modelling framework: simulation and evaluation of water and resource recovery

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Summary

Desalination plays a crucial role in addressing the growing challenges of water scarcity. In recent years, the integration of desalination and brine treatment technologies has been increasingly studied, aiming to develop sustainable solutions for resource recovery from seawater. However, designing treatment trains and optimizing these processes for maximum efficiency, sustainability, and cost-effectiveness are complex tasks that require data, sophisticated analysis and decision-making strategies. Our software offers a comprehensive modelling framework for simulating desalination and mineral recovery systems. Integrating technical process models with economic and environmental analysis provides valuable insights into the integration of these technologies and their impact on production efficiency, energy consumption, and environmental performance. Through our software's simulations, researchers, engineers, and policymakers gain the power to evaluate the resource recovery potential, economics, and greenhouse gas emissions associated with different configuration combinations. This empowerment with crucial information for early-stage design and strategic planning is a significant step toward fostering more sustainable water management practices.

Statement of need

Traditionally, simulation models were developed to evaluate the influence of certain parameters on the characteristics of the recovered products and the performance of the technology in terms of energy, chemicals, and water consumption. However, in the desalination field, open-access simulation tools are notably lacking. While commercial software programs, like WAVE ([Dupont, 2024](#)), exist for membranes, and numerous publications discuss techno-economic models for desalination ([El-Dessouky & Ettouney, 2002](#)) and brine treatment technologies ([Chen et al., 2021](#); [Micari et al., 2020](#); [Morgante et al., 2022](#); [Panagopoulos, 2021](#); [Poirier et al., 2022](#); [Dimitrios Xevgenos et al., 2015](#)), there is a noticeable absence of open-access simulation tools in the literature. The WaterTAP platform ([Energy, 2024](#)) offers an open-source library for modelling water treatment technologies like reverse osmosis and electrodialysis. While it provides valuable simulation capabilities, it mainly focuses on desalination technologies and lacks several important brine treatment technologies such as chemical precipitation and

crystallization.

With the shift towards circular systems and integrated desalination and brine treatment technologies for resource recovery, there is a need for a unified tool. Our software, Desalsim addresses this need by integrating a diverse range of technologies—reverse osmosis, nanofiltration, multi-effect distillation, chemical precipitation, eutectic freeze crystallization, electrodialysis, and thermal crystallization—into a comprehensive platform. This platform not only models these processes but also provides detailed techno-economic and environmental analyses.

Though WaterTAP is powerful, it requires considerable expertise in Python programming and numerical methods. Desalsim is designed to be more accessible, making it easier for researchers without advanced programming skills to perform simulations and analyze results. This ease of use makes Desalsim particularly valuable for researchers exploring desalination and brine treatment technologies. It is especially useful when detailed techno-economic and environmental assessments are required. The software provides a variety of examples to help modellers design and evaluate different technical configurations.

By offering transparent and accessible models, DesalSim aims to enhance the credibility, repeatability, and comparability of desalination studies, supporting informed design and decision-making in the field of desalination and resource recovery.

Limitations

The proposed software is not designed to replace detailed physical models or system dynamics approaches. For applications requiring highly detailed process representations, the software may need to be enhanced to provide more detailed results and optimization opportunities. This work highlights that the proposed software is particularly valuable for evaluating the integration of different processes and preliminary designs, capturing the technical, economic, and environmental impacts of technology integration.

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The technical process models were developed based on the report from (D. Xevgenos et al., 2023) and the following literature (Cassaro et al., 2023; Morgante et al., 2022; Nayar et al., 2019). Then they were validated with experimental results from (Morgante et al., 2024). The development of economic models were influenced by (Abraham & Luthra, 2011; Bilton et al., 2011; Choi et al., 2015; Kesime et al., 2013; Peters & Timmerhaus, 2003). The analysis and comparison were developed based on (Ktori et al., 2024). Detailed mathematical descriptions of the simulation equations and economic models are provided in the [Mathematical Description](#).

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