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

Rodoula Ktori[1], Fabrizio Vassallo[2], Giovanni Virruso[2], Carmelo Morgante[2], Andrea Culcasi[2], Dionysia Diamantidou[3], Niels Van Linden[3], Alessandro Trezzi[4], Adithya Krishnan[5], Andrea Cipollina[2], Giorgio Micale[2], Mark C. M. van Loosdrecht[1], and Dimitrios Xevgenos[6]

1 Department of Biotechnology, Delft University of Technology, Van der Maasweg 9, 2629 HZ, Delft, The Netherlands **2** Dipartimento di Ingegneria, Università degli Studi di Palermo - viale delle Scienze Ed.6, 90128 Palermo, Italy **3** Lenntech BV, Distributieweg 3, 2645 EG Delfgauw, The Netherlands **4** Sofinter S.p.A, Piazza Francesco Buffoni, 3, 21013 Gallarate VA, Italy **5** Water & Energy Intelligence BV, the Netherlands **6** Technology Policy & Management faculty, Delft University of Technology, Jaffalaan 5, 2628 BX Delft, The Netherlands

DOI: 10.21105/joss.07062

Software

- Review
- Repository
- Archive

Editor: Jayaram Hariharan

Reviewers:

- @rkingsbury
- @yalinli2
- @BenWinchester

Submitted: 10 May 2024
Published: 17 December 2024

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.

Acknowledgements

The software was developed by Rodoula Ktori, with theoretical support from all co-authors. Technological experts conducted the validation of each simulation model for the respective technology: Nanofiltration: Dionysia Diamantidou, Niels van Linden; Multi-effect Distillation: Alessandro Trezzi; MF-PFR: Fabrizio Vassallo, Carmelo Morgante, Andrea Cipollina; EDBM: Giovanni Virruso, Andrea Culcasi; EFC: Marcos Rodriguez Pascual.

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; Kesieme 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.

This work was supported by the EU within the WATER MINING (Next generation water-smart management systems: large scale demonstrations for a circular economy and society) - Horizon 2020 research and innovation programme under grant agreement No 869474.

References

Abraham, T., & Luthra, A. (2011). Socio-economic & technical assessment of photovoltaic powered membrane desalination processes for india. *Desalination*, *268*(1-3), 238–248. https://doi.org/10.1016/j.desal.2010.10.035

Bilton, A. M., Wiesman, R., Arif, A., Zubair, S. M., & Dubowsky, S. (2011). On the feasibility of community-scale photovoltaic-powered reverse osmosis desalination systems for remote locations. *Renewable Energy*, *36*(12), 3246–3256. https://doi.org/10.1016/j.renene.2011.03.040

Cassaro, C., Virruso, G., Culcasi, A., Cipollina, A., Tamburini, A., & Micale, G. (2023). Electrodialysis with bipolar membranes for the sustainable production of chemicals from seawater brines at pilot plant scale. *ACS Sustainable Chemistry & Engineering*, *11*(7), 2989–3000. https://doi.org/10.1021/acssuschemeng.2c06636

Chen, Q., Burhan, M., Shahzad, M. W., Ybyraiymkul, D., Akhtar, F. H., Li, Y., & Ng, K. C. (2021). A zero liquid discharge system integrating multi-effect distillation and evaporative crystallization for desalination brine treatment. *Desalination*, *502*, 114928. https://doi.org/10.1016/j.desal.2020.114928

Choi, Y., Cho, H., Shin, Y., Jang, Y., & Lee, S. (2015). Economic evaluation of a hybrid desalination system combining forward and reverse osmosis. *Membranes*, *6*(1), 3. https://doi.org/10.3390/membranes6010003

Dupont. (2024). *WAVE water treatment design software*. https://www.dupont.com/water/resources/design-software.html

El-Dessouky, H. T., & Ettouney, H. M. (2002). *Fundamentals of salt water desalination*. Elsevier. https://doi.org/10.1016/B978-0-444-50810-2.50018-X

Energy, U. S. Dept. of. (2024). *WaterTAP: An open-source water treatment model library (version 0.6)*. https://github.com/watertap-org/watertap

Kesieme, U. K., Milne, N., Aral, H., Cheng, C. Y., & Duke, M. (2013). Economic analysis of desalination technologies in the context of carbon pricing, and opportunities for membrane distillation. *Desalination*, *323*, 66–74. https://doi.org/10.1016/j.desal.2013.03.033

Ktori, R., Parada, M. P., Rodriguez-Pascual, M., Loosdrecht, M. C. van, & Xevgenos, D. (2024). A value-sensitive approach for integrated seawater desalination and brine treatment. *Sustainable Production and Consumption*. https://doi.org/10.1016/j.spc.2024.11.006

Micari, M., Cipollina, A., Tamburini, A., Moser, M., Bertsch, V., & Micale, G. (2020). Techno-economic analysis of integrated processes for the treatment and valorisation of neutral coal mine effluents. *Journal of Cleaner Production*, *270*, 122472. https://doi.org/10.1016/j.jclepro.2020.122472

Morgante, C., Vassallo, F., Cassaro, C., Virruso, G., Diamantidou, D., Van Linden, N., Trezzi, A., Xenogianni, C., Ktori, R., Rodriguez, M., & others. (2024). Pioneering minimum liquid discharge desalination: A pilot study in lampedusa island. *Desalination*, 117562. https://doi.org/10.1016/j.desal.2024.117562

Morgante, C., Vassallo, F., Xevgenos, D., Cipollina, A., Micari, M., Tamburini, A., & Micale, G. (2022). Valorisation of SWRO brines in a remote island through a circular approach: Techno-economic analysis and perspectives. *Desalination*, *542*, 116005. https://doi.org/10.1016/j.desal.2022.116005

Nayar, K. G., Fernandes, J., McGovern, R. K., Dominguez, K. P., McCance, A., Al-Anzi, B. S., & others. (2019). Cost and energy requirements of hybrid RO and ED brine concentration systems for salt production. *Desalination*, *456*, 97–120. https://doi.org/10.1016/j.desal.2018.11.018

Panagopoulos, A. (2021). Beneficiation of saline effluents from seawater desalination plants: Fostering the zero liquid discharge (ZLD) approach-a techno-economic evaluation. *Journal of Environmental Chemical Engineering*, *9*(4), 105338. https://doi.org/10.1016/j.jece.2021.105338

Peters, M. S., & Timmerhaus, K. D. (2003). *Plant design and economics for chemical engineers*

(5th ed.). McGraw-Hill Chemical Engineering Series.

Poirier, K., Al Mhanna, N., & Patchigolla, K. (2022). Techno-economic analysis of brine treatment by multi-crystallization separation process for zero liquid discharge. *Separations*, *9*(10), 295. https://doi.org/10.3390/separations9100295

Xevgenos, D., Ktori, R., Gils, E. van, Diamantidou, D., Linden, N. van, Vassalo, F., Morgante, C., Culcasi, A., Rodrigues Pascual, M., Avramidi, M., Trezzi, A., Krishnan, A., Nauta, J. T., Cipollina, A., & Micale, G. (2023). *Deliverable 3.1 report on the design procedure including bench-scale tests for CS1 and CS2*. https://www.watermining.eu

Xevgenos, Dimitrios, Michailidis, P., Dimopoulos, K., Krokida, M., & Loizidou, M. (2015). Design of an innovative vacuum evaporator system for brine concentration assisted by software tool simulation. *Desalination and Water Treatment*, *53*(12), 3407–3417. https://doi.org/10.1080/19443994.2014.948660