Simulation and optimization of CCRO systems and associated water networks

Authors: Pedro Henrique Callil-Soares; Galo Antônio Carrillo Le Roux; René Peter Schneider*

Chemical Engineering Department, Polytechnic School of the University of São Paulo

Corresponding Author: *schneiderpqi@usp.br

Abstract

Water network systems are ubiquitous in many engineering areas, and their association with water purification technologies is essential to urban water distribution. Closed-circuit reverse osmosis (CCRO), is a new technology for water purification, employing a membrane system under a cyclic steady-state regime. However, despite the availability of several models for network design/optimization, and for membrane systems simulation, there are none that can be applied to brazilian systems, since no network models implement legal requirements for well downtime and no membrane simulator includes crystallization kinetics, leading to infeasible/suboptimal solutions.

In this study, we formulated new models and implemented Python libraries for optimization of water networks (including well downtime requirements), and for reverse osmosis plant simulation. For networks, we used a multiple-shooting approach for discretization and disjunctive programming constraints for downtime and its contiguity[1]; bilinearities were linearized with logarithmic decomposition[2]. We implemented each unit (wells, plants, etc.) as a class, with a library being written to program units and their integration, allowing users to model generic networks. For plants, a system of partial differential-algebraic equations[3] was coupled with precipitation kinetics for efficiency assessment and operation optimization, and we programmed an implementation of this model as another library. Both libraries will be published in the near future.

We applied our models to the optimization of the water distribution system of a city in São Paulo state, where wells with high Fluoride concentrations preclude simple mixing solutions to achieve acceptable water quality. There, new optimization options were revealed: rerouting certain streams and replacing the current system with a CCRO plant would allow all constraints to be met and decrease discharges by 65%, showcasing the models' capacity to yield efficient schedule and design options.

Keywords

CCRO, network optimization, water networks, membrane modelling

Acknowledgements

Grant 2023/04683-7, São Paulo Research Foundation (FAPESP).

References

[1] S. Kolodziej, P. M. Castro, & I. E. Grossmann. Global optimization of bilinear programs with a multiparametric disaggregation technique. *Journal of Global Optimization, 57*, 1039-1063, 2013

[2] L. T. Biegler, I. E. Grossmann, & A. W. Westerberg: Systematic methods for chemical process design, 1997

[3] M. Li. Cyclic simulation and energy assessment of closed-circuit RO (CCRO) of brackish water. *Desalination, 545*, 116149, 2023