Integrating the Design of Desalination Technologies into Produced Water Network Optimization

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ABSTRACT

The oil and gas energy sector uses billions of gallons of water for hydraulic fracturing each year to extract oil and gas. The water injected into the ground for fracturing along with naturally occurring formation water from the oil wells surfaces back in the form of produced water. Produced water can contain high concentrations of total dissolved solids and is unfit for reuse outside the oil and gas industry without desalination. In semi-arid shale plays, produced water desalination for beneficial reuse could play a crucial role in alleviating water shortages and addressing extreme drought conditions. In this paper we co-optimize the design and operation of desalination technologies along with operational decisions across produced water networks. A multi-period produced water network model with simplified split-fraction-based desalination nodes is developed. Rigorous steady-state desalination mathematical models based on mechanical vapor recompression are developed and embedded at the desalination sites in the network model. An optimal common design is ensured across all periods using global capacity constraints. The solution approach is demonstrated for multi-period planning problems on networks from the PARETO open-source library. Model formulation and challenges associated with scalability are discussed.

Keywords: Water Networks, Process Design, Modelling, Pyomo, Optimization

1 INTRODUCTION

Hydraulic fracturing accounts for about half of current US crude oil production [1]. It involves the injection of large volumes of water underground to build pressure and force open rocks to release underground oil and gas reserves. The injected water along with natural formation water is returned to the surface as shown in Figure 1 and contains dissolved solids, oil, grease, and chemicals used during the well stimulation. The volume and quality of the water varies over time and is different from well to well. The oil and gas industry produces billions of gallons of high total dissolved solids (TDS) produced water every year due to oil and gas operations. There is a need to manage that water in cost-efficient and environmentally sustainable ways.

Currently, produced water is either disposed or recycled for well development purposes with pre-treatment by adding friction reducers or other chemicals. Strategic planning and optimal operational policies in produced water management have shown to increase water reuse within the oil and gas industry, making the process more sustainable [2-3]. Several efforts have focused on building infrastructure for produced water management for economic and environmental benefits. For example, optimization models that minimize the cost of produced water management have been developed that consider reuse, storage and simplified treatment [4]. Multi-period planning models involving network infrastructure expansion and strategic decisions have been shown to significantly improve profitability for upstream operators [5]. Due to large quantities of produced water and fracking scheduling, it may not be feasible to recycle a 100% of produced water within the oil and gas industry [6].

To reuse produced water outside the oil and gas industry, it requires extensive treatment (i.e., desalination) to bring its quality to acceptable levels by lowering TDS concentrations. Desalination technologies for produced water are mainly classified into thermal-based [7–9] and

membrane-based [10-11] technologies. Several studies have focused on developing detailed mathematical models for the desalination units to develop techno-economic analyses and determine the effectiveness of different desalination technologies [12–14]. Multi-effect evaporation with mechanical vapor recompression (MEE-MVR) is a potential desalination technology for produced water at an industrial scale [7]. A thermo-economic model for an MEE-MVR process has been developed in [15]. Also, detailed nonlinear programming (NLP) models for the MEE-MVR process were developed in [16] with heat integration for the desalination of produced water from shale gas plays. These models were further used to minimize the total annualized cost (TAC) of the desalination unit and determine the optimal design and operation given the feed flow and salinity of produced water.

Figure 1: Hydraulic fracturing
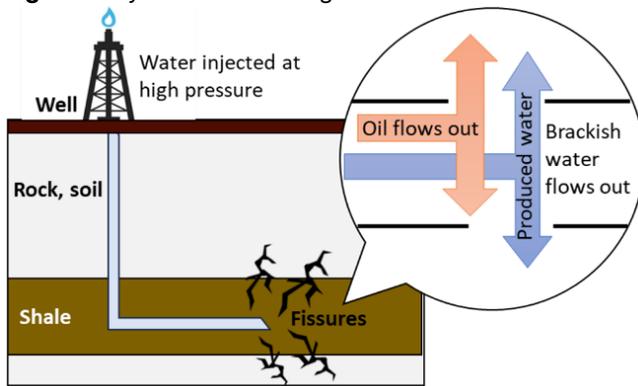
Although produced water network optimization and optimization of rigorous desalination units have been individually explored, there is a gap with respect to integrating these two research areas to create an overall optimal decision-making system. In [12] a network optimization model was developed for the Marcellus shale play by using a treatment cost model, obtained using techno-economic assessment of membrane distillation. Simplified costing models for treatment have been used in several works which consider produced water management optimization [2, 4]. However, these formulations don't provide the optimal treatment system design and operational decisions of the treatment units.

This work supports the development of PARETO – a DOE-sponsored, free, and open-source optimization framework for onshore produced water management (www.project-pareto.org), by integrating detailed desalination models into the existing produced water management framework. Specifically, in this paper, we introduce a formulation for integrating steady-state desalination units into multi-period produced water network models for the co-optimization of design and operational decisions. A multi-period produced water network model consisting of production pads, completion pads, storage, disposal, and desalination units has been developed.

Since the resulting integrated formulation is nonlinear, it is crucial to ensure that there are no singularities arising due to zero flows in the network. Therefore, separate flow variables for solid and liquid flows are used for the mass balances to avoid bilinear terms in each network arc. We use the MEE-MVR model [16] with heat integration for the rigorous desalination unit with a separate MEE-MVR model for each period. A common design is ensured across all periods using global capacity constraints on the design variables. In Section 2 we provide the mathematical formulation for the produced water network model, desalination units, and the integrated problem. Section 3 consists of case studies on a multi-period network with integrated desalination models. Section 4 concludes the paper with a discussion on scaling up the problem to larger networks.

2 MODEL FORMULATION

Network Model

A typical produced water network consists of production pads (well sites) comprising mature oil or gas wells, which produce hydrocarbons and water, and completion pads, which have a water demand for drilling and hydraulic fracturing. It also consists of disposal wells, storage units, and – in the future – may involve desalination units where excess produced water can be sent. Completions pads' water demand (for hydraulic fracturing) can be met using existing water from the production pads or by procuring fresh water; this depends upon the cost of transportation vs. the cost of sourcing. Figure 2 shows a schematic of a produced water network along with all possible network arcs.
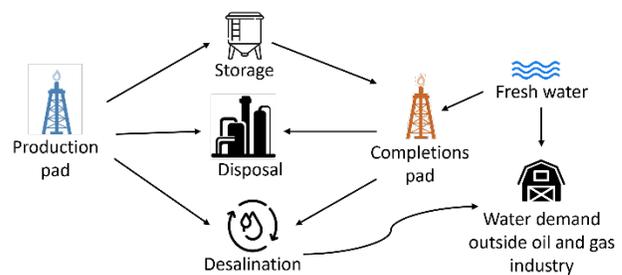

Figure 2: Produced water network.

In this section we describe our model formulation with mass balances for the produced water network model. Table 1 describes all the sets, variables, and parameters used in the formulation.

Table 1: Description of sets, variables, and parameters for the network model.

Sets

$\mathcal{N}^P, \mathcal{N}^C, \mathcal{N}^{MS}$	Production pads, completion pads, mixers, or splitters respectively
$\mathcal{N}^{T,IN}, \mathcal{N}^{T,TW},$ $\mathcal{N}^{T,CW}$	Desalination inlet, treated water, and concentrated water nodes
$\mathcal{T}$	Total time periods
$\mathcal{T}_n^P, \mathcal{T}_n^C, \mathcal{T}_n^0$	Periods when node n is producing, consuming, or neither, respectively
$\mathcal{Q}$	Components in the stream
$\mathcal{A}$	Arcs in the network
$\mathcal{A}_n^{In}$	Arcs to the inlet of node n
$\mathcal{A}_n^{Out}$	Arcs from the outlet of node n
$\mathcal{N}^{Up}(n)$	Upstream node of node n
$a^{In}(n), a^{Out}(n)$	Arcs in or out of node n, respectively
Variables	
F_{at}	Flowrate of water in arc a at time t
S_{aqt}	Flowrate of solids q in arc a at time t
C_{nqt}	Concentration of q at node n at time t
C_{nt}^{total}	Total concentration at node n at time t
I_{nt}	Water in inventory unit n at time t
I_{nqt}^S	Solids q in inventory unit n at time t
α_{nt}	Water recovery fraction at desalination unit n at time t
Parameter	
$\hat{F}_{nt}^{Prod}, \hat{F}_{nt}^{Cons}$	Flowrate of water produced and consumed at node n at time t
$\hat{S}_{nqt}^{Prod}, \hat{S}_{nqt}^{Cons}$	Flowrate of solids q produced and consumed at node n at time t
$\hat{C}_{nqt}^{Prod}$	Concentration of solids q produced at node n at time t
$\hat{I}_n^0$	Initial water inventory at the inventory node
$\hat{I}_n^{s0}$	Initial TDS level at the inventory node
$\hat{C}_{min}^{total}, \hat{C}_{max}^{total}$	Concentration bounds for the desalination inlet stream
$\hat{F}_n^{min}, \hat{F}_n^{max}$	Flowrate bounds for desalination inlet node n
Δt	Time discretization

A general flow balance for water and solids can be written for each network connecting the mixers, splitters, and the production pads:

$$\sum_{a\in\mathcal{A}_n^{In}} F_{at} + \hat{F}_{nt}^{Cons} = \sum_{a\in\mathcal{A}_n^{Out}} F_{at} + \hat{F}_{nt}^{Cons} \quad \forall n \in \mathcal{N}^P \cup \mathcal{N}^{MS}, t \in \mathcal{T}$$

$$\sum_{a\in\mathcal{A}_n^{In}} S_{aqt} + \hat{S}_{nqt}^{Prod} = \sum_{a\in\mathcal{A}_n^{Out}} S_{aqt} + \hat{S}_{nqt}^{Cons} \quad \forall n \in \mathcal{N}^P \cup \mathcal{N}^{MS}, q \in \mathcal{Q}, t \in \mathcal{T}$$

The outlet lines of the splitters contain equal concentration of solids. This constraint can be expressed as:
If $|\mathcal{A}_n^{Out}| > 1$,

$$\hat{S}_{iqt} \sum_{a\in\mathcal{A}_n^{In}} F_{at} = F_{it} \sum_{a\in\mathcal{A}_n^{In}} S_{aqt} \quad \forall i \in \mathcal{A}_n^{Out}, n \in \mathcal{N}^{MS}, q \in \mathcal{Q}, t \in \mathcal{T}$$

For the inventory nodes, the mass balance is given by:

$$I_{nt} = I_{nt-1} + \sum_{a\in\mathcal{A}_n^{In}} F_{at} - \sum_{a\in\mathcal{A}_n^{Out}} F_{at} \quad \forall n \in \mathcal{N}^S, t \in \mathcal{T}$$

If there is a pretreatment unit installed before the inventory node, the concentration of solids in the inventory is zero. Otherwise, a solids mass balance is required to track the concentration of solids in the inventory:

$$I_{nqt}^S = I_{nqt-1}^S + \sum_{a\in\mathcal{A}_n^{In}} S_{aqt} - \sum_{a\in\mathcal{A}_n^{Out}} S_{aqt} \quad \forall n \in \mathcal{N}^S, q \in \mathcal{Q}, t \in \mathcal{T}$$

The solids flow out of the inventory, depend on the concentration of the stored water and are given by:

$$S_{aqt} = F_{at} C_{nqt} \quad , \quad C_{nqt} I_{nt} = I_{nqt}^S \quad \forall n \in \mathcal{N}^S, q \in \mathcal{Q}, t \in \mathcal{T}$$

Completions pads can consume water, produce water, do both simultaneously, or neither produce nor have demand. Depending upon the mode of operation, the completions pad mass balances need to be written differently. If the completions pad is consuming water:

$$\hat{F}_{nt}^{Cons} = \sum_{a\in\mathcal{A}_n^{In}} F_{at} \quad \forall n \in \mathcal{N}^C, t \in \mathcal{T}_n^C$$

$$\sum_{a\in\mathcal{A}_n^{Out}} F_{at} = 0, \sum_{a\in\mathcal{A}_n^{Out}} S_{aqt} = 0 \quad \forall n \in \mathcal{N}^C, q \in \mathcal{Q}, t \in \mathcal{T}_n^C$$

If the completions pad is producing water:

$$\hat{F}_{nt}^{Prod} = \sum_{a\in\mathcal{A}_n^{Out}} F_{at} \quad \forall n \in \mathcal{N}^C, t \in \mathcal{T}_n^P$$

$$\hat{S}_{nqt}^{Prod} = \sum_{a\in\mathcal{A}_n^{Out}} S_{aqt} \quad \forall n \in \mathcal{N}^C, t \in \mathcal{T}_n^P, q \in \mathcal{Q}$$

$$\sum_{a\in\mathcal{A}_n^{In}} F_{at} = 0, \sum_{a\in\mathcal{A}_n^{In}} S_{aqt} = 0 \quad \forall n \in \mathcal{N}^C, q \in \mathcal{Q}, t \in \mathcal{T}_n^P$$

If the completions pad is simultaneously producing and consuming:

$$\hat{F}_{nt}^{Prod} = \sum_{a\in\mathcal{A}_n^{Out}} F_{at}, \hat{F}_{nt}^{Cons} = \sum_{a\in\mathcal{A}_n^{In}} F_{at} \quad \forall n \in \mathcal{N}^C, t \in \mathcal{T}_n^{PC}$$

$$\hat{S}_{nqt}^{Prod} = \sum_{a\in\mathcal{A}_n^{Out}} S_{aqt} \quad \forall n \in \mathcal{N}^C, t \in \mathcal{T}_n^{PC}, q \in \mathcal{Q}$$

If the completions pad is neither consuming nor producing water:

$$\sum_{a\in\mathcal{A}_n^{In}} F_{at} = 0, \qquad \sum_{a\in\mathcal{A}_n^{Out}} F_{at} = 0 \quad \forall n \in \mathcal{N}^C, t \in \mathcal{T}_n^0$$

$$\sum_{a\in\mathcal{A}_n^{In}} S_{aqt} = 0, \qquad \sum_{a\in\mathcal{A}_n^{In}} S_{aqt} = 0 \quad \forall n \in \mathcal{N}^C, q \in \mathcal{Q}, t \in \mathcal{T}_n^0$$

The desalination unit node in the network is broken down into three parts: the inlet node, the concentrated water node, and the treated water node. For the desalination inlet node, we ensure that there is only one inlet connection. If there are multiple inlet lines going into a desalination unit, we add a mixer node with one outlet that goes to the desalination unit. The desalination inlet node equations are given by:

$$C_{nt}^{total} \sum_{a\in\mathcal{A}_n^{In}} F_{at} = \sum_{q\in\mathcal{Q}} \sum_{a\in\mathcal{A}_n^{In}} S_{aqt} \quad \forall n \in \mathcal{N}^{T,In}, t \in \mathcal{T}$$

The treated water stream from the desalination unit is considered fresh with zero salinity. This assumption is true in the case of MEE-MVR, since the condensate from the evaporators contains negligible amounts of solids. The concentrated water node consists of the brine from the desalination unit. The flow in and flow out are related by the water recovery fraction:

$$F_{a^{Out}(n)t} = \alpha_{n't} F_{a^{In}(n')t} \quad \forall n \in \mathcal{N}^{T,TW}, n' \in \mathcal{N}^{Up}(n), t \in \mathcal{T}$$

$$F_{a^{Out}(n)t} = (1 - \alpha_{n't}) F_{a^{In}(n')t} \quad \forall n \in \mathcal{N}^{T,CW}, n' \in \mathcal{N}^{Up}(n), t \in \mathcal{T}$$

$$C_{nqt} F_{a^{Out}(n)t} = C_{n'qt} F_{a^{In}(n')t}, \quad S_{a^{Out}(n)qt} = C_{nqt} F_{a^{Out}(n)t}$$
$$\forall n \in \mathcal{N}^{T,CW}, n' \in \mathcal{N}^{Up}(n), t \in \mathcal{T}, q \in \mathcal{Q}$$

We assume that the desalination unit has a minimum flow and concentration restriction. This assumption is reasonable as the startup procedure for the desalination units can be time consuming and expensive compared to running them at some minimum capacity for the entire planning horizon. Therefore, the bounds on desalination operation can be written as:

$$\hat{C}_{min}^{total} \leq C_{nt}^{total} \leq \hat{C}_{max}^{total} \quad \forall n \in \mathcal{N}^{T,In}, t \in \mathcal{T}$$

$$\hat{F}_n^{min} \leq \sum_{a \in \mathcal{A}_n^{In}} F_{at} \leq \hat{F}_n^{max} \quad \forall n \in \mathcal{N}^{T,In}, t \in \mathcal{T}$$

The disposal sites also have disposal limits on the volume of water that can be disposed in a particular period:

$$\sum_{a \in \mathcal{A}_n^{In}} F_{at} \leq \hat{F}_n^{max} \quad \forall n \in \mathcal{N}^D, t \in \mathcal{T}$$

We assume that the salinity of the fresh water sourced is near-zero and that there are capacity constraints on the volume of water that can be sourced:

$$\sum_{a \in \mathcal{A}_n^{Out}} F_{at} \leq \hat{F}_n^{max}, \quad \sum_{a \in \mathcal{A}_n^{Out}} S_{aqt} = 0 \quad \forall n \in \mathcal{N}^D, q \in \mathcal{Q}, t \in \mathcal{T}$$

The main advantage of including the solids flow stream into the network model is that we can bound the solids flow when the flow of water in any arc is zero:

$$S_{aqt} \leq \hat{C}^{max} F_{at} \quad \forall a \in \mathcal{A}, q \in \mathcal{Q}, t \in \mathcal{T}$$

This constraint avoids singularities in the problem formulation and improves the robustness of the model while optimizing.

The operating cost of the network includes costs for transportation, storing water in the inventory units, sourcing fresh water, and produced water disposal or injection. The desalination of water and the removal of water from the inventory unit has a reward associated with it to encourage desalination and discourage storage of produced water. The desalination cost comes from the detailed MEE-MVR process model costs and hence is not included in the network cost here:

$$C_{net} = \sum_{t \in \mathcal{T}} \left[\sum_{a \in \mathcal{A}} \beta_{ar} F_{at} + \sum_{n \in \mathcal{N}^S} \sum_{a \in \mathcal{A}_n^{In}} \beta_s F_{at} + \sum_{n \in \mathcal{N}^W} \sum_{a \in \mathcal{A}_n^{Out}} \beta_s F_{at} \right.$$
$$+ \sum_{n \in \mathcal{N}^D} \sum_{a \in \mathcal{A}_n^{In}} \beta_d F_{at} - \sum_{n \in \mathcal{N}^S} \sum_{a \in \mathcal{A}_n^{Out}} \gamma_s F_{at}$$
$$\left. - \sum_{n \in \mathcal{N}^{T,TW}} \sum_{a \in \mathcal{A}_n^{Out}} \gamma_T F_{at} \right] \Delta t$$

Desalination Model

An MEE-MVR process unit consists of single or multiple evaporator stages where the feed water enters on the shell side. As seen in Figure 3, hot steam flows through the evaporator tubes and the resulting heat transfer evaporates the feed water, which is split into liquid brine and vapor streams. In a multistage evaporation setting, the vapor from the ith evaporator is fed into the tubes of the $(i + 1)^{th}$ evaporator and the brine from the ith evaporator is fed into the $(i - 1)^{th}$ evaporator. A compressor is used for vapor recompression from the last evaporator stage to feed it into the tubes of the first evaporator in the sequence. A preheater is used to exchange heat between the condensate and the feed to pre-heat the feed for better energy integration.

A rigorous MEE-MVR process model is developed based on [16], the mathematical model consists of mass and energy balances and non-linear pressure and temperature relationships along with bounds for feasible operation. The detailed modeling equations are provided in the digital supplementary material. The main costs associated with the desalination unit are the CAPEX from the evaporators, preheater, and the compressor and the OPEX from using electricity to run the compressor. The CAPEX was calculated using correlations from [17] and was annualized using an amortization period of 10 years and an interest rate of 10%.
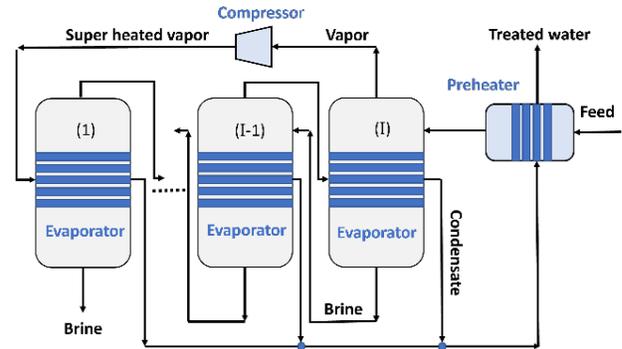

Figure 3. MEE-MVR process with heat integration.

Integrated Model

To formulate the multi-period integrated problem, a steady-state MEE-MVR unit model is written in each period of the network. The variables from the network are linked with the input variables (represented by a bar on top of the variables) to the desalination unit using linking constraints. To ensure a common desalination design across all periods and feasible operation in every period, we use global capacity constraints on the capacity variables of the desalination model. The annualized CAPEX and OPEX are converted to daily CAPEX and OPEX given by $CAPEX_{\Delta t}$ and $OPEX_{\Delta t}$. The integrated model formulation is given by:

$$\min C_{net} + \sum_{t \in \mathcal{T}} (CAPEX_{\Delta t} + OPEX_{\Delta t}^t) \Delta t$$

s.t $\sum_{a \in \mathcal{A}_n^{In}} F_{at} = \bar{F}_{nt}^{in} \quad \forall n \in \mathcal{N}^{T,In}, t \in \mathcal{T}$

$\quad C_{nt}^{total} = \bar{C}_{nt}^{in} \quad \forall n \in \mathcal{N}^{T,In}, t \in \mathcal{T}$

$\quad \alpha_{nt} = \bar{\alpha}_{nt} \quad \forall n \in \mathcal{N}^{T,In}, t \in \mathcal{T}$

$\quad CAPEX_{evap}^{(i)global} \geq \overline{CAPEX}_{evap,t}^{(i)} \quad \forall i \in \{1,..,I\}, t \in \mathcal{T}$

$\quad CAPEX_{ph}^{global} \geq \overline{CAPEX}_{ph,t} \quad \forall\, t \in \mathcal{T}$

$\quad CAPEX_{comp}^{global} \geq \overline{CAPEX}_{comp,t} \quad \forall t \in \mathcal{T}$

*All network equations and desalination model
equations in each period*

The $CAPEX_{\Delta t}$ is calculated using the global CAPEX of individual equipment. It is assumed that there are no uncertainties in the model. The integrated problem is a nonlinear model, developed in Pyomo [18] and solved using the open source NLP solver IPOPT [19].

3 RESULTS

In this section we demonstrate the results of our integrated optimization approach on a small network case study provided by "Project PARETO". The network consists of four production pads, one completions pad, two disposal sites, two fresh water sources, one storage site, and one prospective desalination site as shown in Figure 4. A planning horizon of 52 weeks is considered with a weekly discretization. The completions pad has a water demand between weeks 1 to 12 and weeks 45 and 52. In the remaining time there is completions flowback, which means there is no demand for water within the network during that time. We perform three case studies:

1. Embedding a single-stage MVR at R01
2. Embedding at two-stage MVR at R01
3. Embedding a three-stage MVR at R01

Case Studies

A single-stage desalination unit is embedded at desalination site R01. The problem consists of 6,972 variables, 6,015 equality constraints, and 2,860 inequality constraints. The optimal network operation profiles are shown in Figure 5. When there is no water demand in the network, the desalination unit is run at its maximum capacity as shown in Figure 5b. When there is completions demand, the optimal solution balances recycling and desalination to reduce costs incurred from freshwater sourcing. From Figure 5c, we observe that initially, when there is completions demand, the inventory is depleted to meet the demand, and then there is inventory build-up to meet the completions demand in the later weeks of the year. Finally, at the end of the year the inventory is completely depleted as there is no incentive to store excess water. The optimal solution indicates that 53% produced water is sent to desalination, 14% is reused to meet completions demand, and 33% is sent to disposal. 4.2 million

barrels of fresh water are sourced to meet the completions demand. Table 2 shows the optimal design variables for the desalination plant.
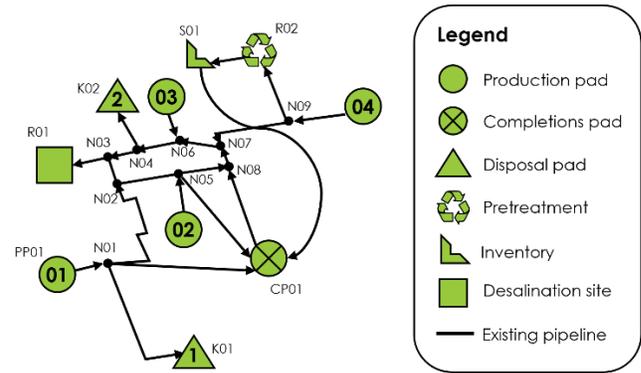

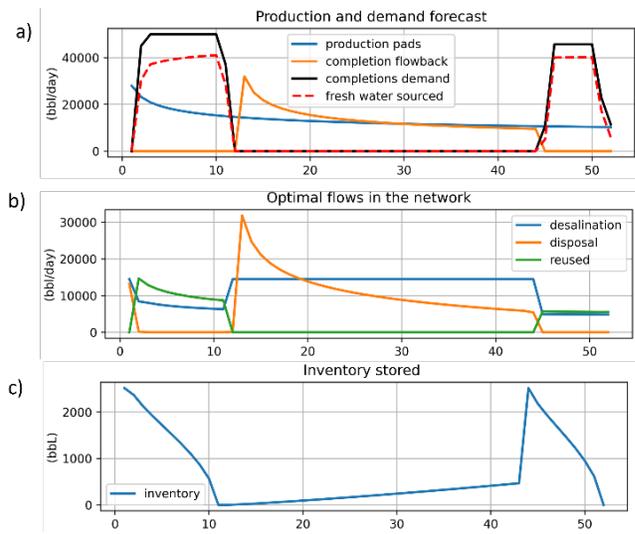**Figure 4.** Produced water network case study.

Figure 5. Optimal flow profiles for a single-stage desalination unit at R01. A) Production and demand forecasts against time and fresh water sourced in each period. b) Optimal water disposal, desalination, and reuse in each time period. c) Optimal volume of water stored in S01 in each period.

When a two-stage desalination unit is embedded at R01, the problem has 8,064 variables, 7,055 equality constraints, and 3,328 inequality constraints. The optimal flow profiles obtained are nearly identical to the single-stage unit. The optimal design variables for the two-stage desalination plant are shown in Table 2. The two-stage desalination plant needs a smaller compressor due to the separation process being split over two evaporator stages. Hence, the CAPEX and the OPEX are both smaller for a two-stage unit compared to a single-stage unit. Overall, the network with a two-stage desalination unit is 31% cheaper than with a single-stage unit in this example.

When a three-stage unit is installed, the desalination

unit doesn't run at its full capacity because the compressor reaches its maximum compression ratio at a lower inlet flowrate to the desalination unit. Thus, the water sent to desalination is decreased, with only 48% water sent to desalination compared to the two-stage and single-stage case. Also, a smaller compressor is installed but the cost of installing three evaporator stages offsets the cost reduction obtained by installing the smaller compressor. Table 3 shows the cost breakdown of the network costs and desalination costs for each case study. Overall, the two-stage desalination unit has the smallest objective function and is therefore optimal in this case. All problems solve with IPOPT within an order of 100 s.

Table 2: Optimal design of the desalination units obtained by solving the integrated problem.

Unit type → Equipment ↓	Single-stage	Two-stage	Three-stage
Evaporator area 1	$372\ m^2$	$372\ m^2$	$372\ m^2$
Evaporator area 2	–	$372\ m^2$	$372\ m^2$
Evaporator area 3	–	–	$372\ m^2$
Preheater area	$73.87\ m^2$	$118\ m^2$	$78\ m^2$
Compressor capacity	$2750\ Hp$	$1790\ Hp$	$1449\ Hp$

Table 3: Optimal costs obtained by solving the integrated problem.

Unit type → Costs (kUSD) ↓	Single-stage	Two-stage	Three-stage
Objective function	9882.9	9094	9575
Transportation	370	370	366
Storage	5.8	5.03	6.12
Disposal	917.5	918	1060
Fresh water	12682	12684	12680
Desalination CAPEX	406	374.8	388
Desalination OPEX	2143.2	1384.2	1075
Storage reward	0.58	0.50	0.61
Desalination reward	6640.6	6641.7	6002

4 CONCLUSIONS

In this paper, we develop an integrated optimization framework for the co-optimization of desalination units with operational decision-making in produced water networks. The framework is demonstrated on a multi-period network problem with three case studies embedding MVR desalination units with different number of stages into the network. The results show that in this case, a two-stage MVR leads to the lowest objective function. The framework gives the optimal operation variables in the network along with the optimal design and operation variables in the rigorous desalination units.

Future work involves developing decomposition techniques for scaling the framework for application on larger network instances. We also plan on incorporating bi-directional flow and strategic decision making into the network model.

DIGITAL SUPPLEMENTARY MATERIAL

The detailed desalination unit model for MEE-MVR process is provided:
https://pareto.readthedocs.io/en/latest/model_library/water_treatment/index.html

ACKNOWLEDGEMENTS

REFERENCES

1. Troy Cook, Jack Perrin. https://www.eia.gov/todayinenergy/detail.php?id=25372
2. Markus Drouven, Andrés Caldéron, Miguel Zamarripa, and Keith Beattie. PARETO: An opensource produced water optimization framework. *Optimization and Engineering*, vol 24. pp. 2229-2249 (2022)
3. Tania Itzel, Serrano-Areválo, Luis Fernando, Lira-Barragán, Mahmoud El-Halwagi, and José María Ponce-Ortega. Strategic Planning for Optimal Management of Different Types of Shale Gas Wastewater. *ACS Sustainable Chem. Eng.*, vol. 10, no. 4, pp. 1451–1470 (2022)
4. Linlin Yang, Ignacio Grossmann, and Jeremy Manno. Optimization models for shale gas water management. *AIChE Journal*, vol. 60, no. 10, pp. 3490–3501 (2014)
5. Markus Drouven and Ignacio Grossmann. Multi-period planning, design, and strategic models for

long-term, quality-sensitive shale gas development. *AIChE Journal*, vol. 62, no. 7, pp. 2296–2323 (2016)

6. Bohyun Hwang, Joonghyeok Heo, Chungwan Lim, Joonkyu Park. Environmental Implications of Shale Gas Hydraulic Fracturing: A Comprehensive Review on Water Contamination and Seismic Activity in the United States. *Water,* vol 15 (2023)

7. Devin Shaffer, Laura Arias Chavez, Moshe Ben-Sasson, Santiago Romero-Vargas Castrillón, Ngai Yin Yip, and Menachem Elimelech. Desalination and Reuse of High-Salinity Shale Gas Produced Water: Drivers, Technologies, and Future Directions. *Environ. Sci. Technol.*, vol. 47, no. 17, pp. 9569–9583 (2013)

8. Alba Carrero-Parreño, Viviani Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, José Caballero, and Juan Reyes-Labarta. Optimization of multistage membrane distillation system for treating shale gas produced water. *Desalination*, vol. 460, pp. 15–27, (2019)

9. Viviani Onishi, Eric Fraga, Juan Reyes-Labarta, and José Caballero. 12 - Desalination of shale gas wastewater: Thermal and membrane applications for zero-liquid discharge In: Emerging Technologies for Sustainable Desalination Handbook pp. 399–431. Ed: Veera Gnaneswar Gude. Elsevier (2018)

10. Nur'Aishah Shahrim, Nada Abounahia, Aya El-Sayed, Haleema Saleem, and Syed Zaidi. An overview on the progress in produced water desalination by membrane-based technology. *Journal of Water Process Engineering*, vol. 51, p. 103479 (2023)

11. Elmira Shamlou, Radisav Vidic, and Vikas Khanna. Optimization-based technoeconomic comparison of multi-stage membrane distillation configurations for hypersaline produced water desalination. *Desalination*, vol. 543, p. 116098 (2022)

12. Sakineh Tavakkoli, Omkar Lokare, Radisav Vidic, and Vikas Khanna. A techno-economic assessment of membrane distillation for treatment of Marcellus shale produced water. *Desalination*, vol. 416, pp. 24–34 (2017)

13. Raquel Salcedo-Díaz, Rubén Ruiz-Femenia, Alba Carrero-Parreño, Viviani Onishi, Juan Reyes-Labarta, and José Caballero. Combining Forward and Reverse Osmosis for Shale Gas Wastewater Treatment to Minimize Cost and Freshwater Consumption In: *Computer Aided Chemical Engineering*, vol. 40, vol. 40. Ed: Antonio Espuña, Moisès Graells, Luis Puigjaner. Elsevier, pp. 2725–2730. (2017)

14. Viviani Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Alba Carrero-Parreño, Juan Reyes-Labarta, Eric Fraga, José Caballero. Process optimization for zero-liquid discharge desalination of shale gas flowback water under uncertainty. *Journal of Cleaner Production*, vol. 164, pp. 1219–1238, (2017)

15. A. S. Nafey, H. E. S. Fath, and A. A. Mabrouk. Thermoeconomic design of a multi-effect evaporation mechanical vapor compression (MEE–MVC) desalination process. *Desalination*, vol. 230, no. 1, pp. 1–15 (2008)

16. Viviani Onishi, Alba Carrero-Parreño, Juan Reyes-Labarta, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Eric Fraga. Shale gas flowback water desalination: Single vs multiple-effect evaporation with vapor recompression cycle and thermal integration. *Desalination*, vol. 404, pp. 230–248 (2017)

17. James Couper, W. Roy Penney, James Fair, and Stanley Walas. Chemical Process Equipment: Selection and Design. Elsevier (2005)

18. William Hart, Jean-Paul Watson, and David Woodruff. Pyomo: modeling and solving mathematical programs in Python. *Mathematical Programming Computation*, vol. 3, no. 3, pp. 219–260 (2011)

19. Andreas. Wächter, Lorenz. T. Biegler. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming, Math. Programming, vol 106, pp. 25-57 (2004)