Systems & Control Transactions

Research Article
Foundations of Computer Aided Process Design (FOCAPD 2024)
Breckenridge, Colorado, USA. July 14-18, 2024
Peer Reviewed Conference Proceeding

An Update on Project PARETO - New Capabilities in DOE's Produced Water Optimization Framework

Miguel A. Zamarripa[a,b]*, Elmira Shamlou[a,b], Javal Vyas[a,b], Travis Arnold[a,b], Philip Tominac[a,b], Melody H. Shellman[a,b], and Markus Drouven[a]

[a] National Energy Technology Laboratory, Pittsburgh, PA, USA
[b] NETL Support Contractor, Pittsburgh, PA, USA
* Corresponding Author: Miguel.Zamarripa-Perez@netl.doe.gov

ABSTRACT

Managing oil and gas produced water, characterized by hypersalinity and large volumes, presents significant challenges. This paper introduces an advanced optimization framework, PARETO, which offers a novel approach to strategic water management, emphasizing produced water (PW) treatment, quality tracking, quantification of emissions, and environmental justice. This work presents a case study showcasing different produced water management challenges. The PARETO framework demonstrated its effectiveness in optimizing water management strategies in line with environmental sustainability and regulatory compliance.

Keywords: produced water management, MINLP, process design, network optimization, MILP

INTRODUCTION

Produced water (PW) management presents significant challenges to oil and gas industry stakeholders due to variable production volumes (unpredictable handling requirements) and water quality, especially due to its high concentrations of total dissolved solids (TDS) and other constituents (necessitating treatment). Given the variability in water produced across different basins along with the difficulty of treating hypersaline brine, oil and gas companies need to identify fit-for-purpose produced water management, treatment, and reuse approaches. Projected increases in PW volumes in coming decades [1], recent injection capacity curtailments [2 - 3], and intensive capital investments (e.g., PW infrastructure) all motivate novel, cost-effective strategies for PW management. Therefore, decision-support tools to assess techno-economic feasibility are critical. However, few such software tools currently exist.

In 2021, the US Department of Energy (DOE) launched a three-year, $5 million PW optimization initiative to develop, demonstrate and deploy PARETO, a novel optimization framework for PW management and beneficial reuse. PARETO is developed by the National Energy Technology Laboratory (NETL), in cooperation with Lawrence Berkeley National Laboratory (LBNL), Carnegie Mellon University, Georgia Tech, New Mexico State University, and the Ground Water Protection Council, and is designed to identify cost-effective and environmentally sustainable PW management, treatment and reuse solutions [4]. Specifically, PARETO supports decision-makers with 1) PW management, including infrastructure buildout recommendations and the coordination of PW deliveries; 2) PW treatment, including treatment facility placement recommendations and the selection of effective treatment technologies; and 3) PW beneficial reuse, including the identification of beneficial reuse options and the distribution of treated PW and/or concentrated brine.

In previous versions of PARETO, the tool's core capabilities for optimizing water distribution across the network were demonstrated using the Mixed Integer Linear Programming (MILP) method [4]. These capabilities included user-defined treatment site specifications and post-process water quality tracking. The optimization aimed at various objectives, such as minimizing costs or maximizing water recycling within the network. Building upon this work, the current version of PARETO introduces significant enhancements, including new methods for integrating produced water (PW) treatment and quality tracking. This is achieved through surrogate modeling of rigorous desalination models, which capture the impact of water quality and flow rate on treatment costs, utilizing both MILP and Mixed Integer Nonlinear Programming (MINLP) methods. Furthermore, this update includes advanced techniques for quantifying emissions and promoting environmental justice, enabling a detailed analysis of the trade-offs between economic factors and environmental objectives. 1) the PARETO treatment module includes a library of PW desalination technologies that can be used to obtain treated water for use outside oil and gas operations; 2) the PARETO environmental module allows a user to track pollutants generated during produced water operations and provides a tool to bring environmental justice to communities located near oil and gas operations.

The results show PARETO's advanced mathematical modeling capabilities are able to solve large scale water network problems, with an emphasis on complex nonlinearities arising from studying effective formulations for solving water networks with water quality predictions.

CASE STUDY AND PROBLEM STATEMENT

This work presents an industrial-size produced water network based on the Permian Basin (New Mexico and Texas).

The main characteristics of PW networks in this region are the availability of pipelines and limited use of trucking for transport (the opposite is true in some other basins such as the Appalachian). Figure 1 shows a representative PW network, which consists of 14 production pads, 3 completion pads, 5 disposal wells, 4 treatment sites (one of which is for desalination – R03), and 3 treatment technologies (i.e., membrane vapor compression, membrane distillation, and osmotic assisted reverse osmosis). Figures 2-4 show the time-varying nature of the water production forecast and completions demand. The PW forecasts follow an exponential decay pattern, whereas the completions pads demand large amounts of water during specific time windows. Table 1 summarizes the water volumes, as can be seen, the PW forecast exceeds the completions demand, which is typical in PW networks.

The main challenges associated with PW network management are:

- Handling large volumes of produced water during specific time windows. (see Figure 3 and 4)
- High salinity (TDS > 120,000 mg/L) and other constituents (i.e., oil, grease, barium, lithium, etc.).
- Pipeline hydraulics (i.e., pressure drop, pumping stations, etc.).
- Active development in the area requiring infrastructure buildout (i.e., new pipelines, new disposal wells, new treatment plants).
- Selecting appropriate treatment and beneficial reuse alternatives for produced water (if available/applicable).

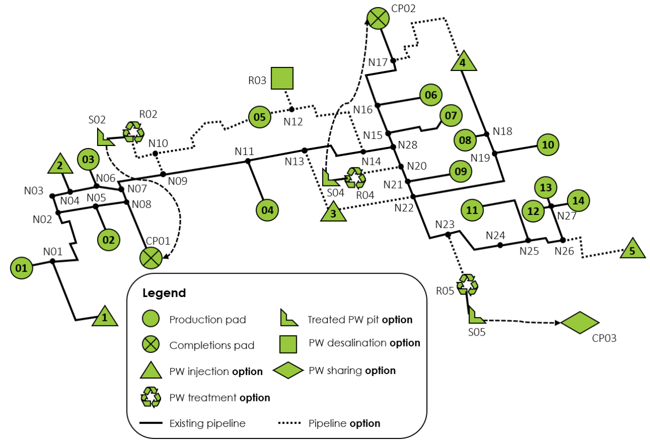

Figure 1: PW network schematic.

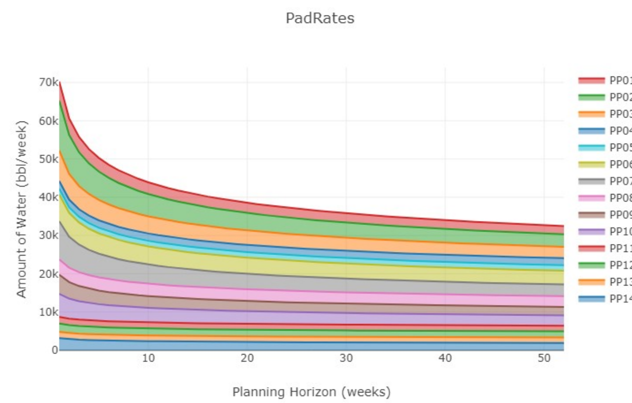

Figure 2: PW forecasts from production pads.

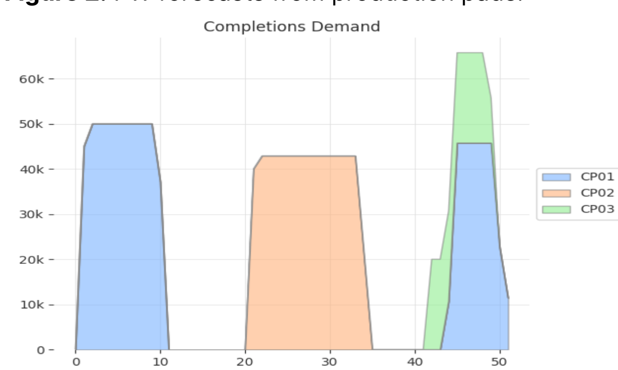

Figure 3: Completions demand volumes.

Figure 4: Flowback forecast from completions pads.

Table 1: Total PW volume and completion demand.

Item	Volume (bbl/day)
Completions Demand	1,481,429
Produced Water Forecast	2,825,953
Disposal Capacity	2,525,714
Starting Treatment Capacity	0

PARETO PRODUCED WATER QUALITY MODELING APPROACH

In produced water network management, a key element involves the estimation of flowrates and water qualities. This process involves tracking various components within the network to efficiently manage and reuse water, tailored to the quality requirements of specific end uses. A notable consideration in modeling these networks is the non-convex and bilinear term in the mass balances emerging from the product of flow rates and concentrations of various components. Within its comprehensive management framework, PARETO adopts two distinct methods to estimate water quality. The main goals are to allow users to: 1) identify component/quality peaks within the produced water network; 2) simulate operating constraints based on water quality limitations; 3) enable the selection and sizing of treatment technologies to enable beneficial reuse.

Quality Post-Processing: In this case, PARETO solves an MILP model focusing on binary decisions and flow rates, without considering water quality. Once these flow rates are estimated, quality constraints are activated and flows and binary variables serve as parameters for subsequent quality assessment, simplifying these calculations to linear constraints. This approach is particularly valuable for pinpointing specific areas in the network that require targeted treatment and for identifying the most suitable technologies for the reuse of produced water (see Figure 5).

Predictive Quality Management: This more advanced method begins with optimizing flow rates using an MILP, followed by the explicit integration of quality constraints. Subsequently, the system is initialized for a comprehensive MINLP model. While this method adeptly sets the stage for detailed analysis, the primary challenge emerges from the intricacies of the bilinear terms, particularly their nonconvex nature. This complexity hampers the achievement of a global optimum, highlighting the advanced analytical challenges inherent in accurately modeling and optimizing such systems. This approach is valuable for adding performance constraints, and/or to identify the best treatment technology for a given network. Figure 5 presents a case study demonstrating the application of an MILP model without quality level restrictions, resulting in elevated quality levels at specific locations. However, by integrating an MINLP model with explicit quality level constraints, it becomes feasible to precisely regulate and monitor the water flow and quality in these areas, ensuring that the quality does not exceed a specified threshold.

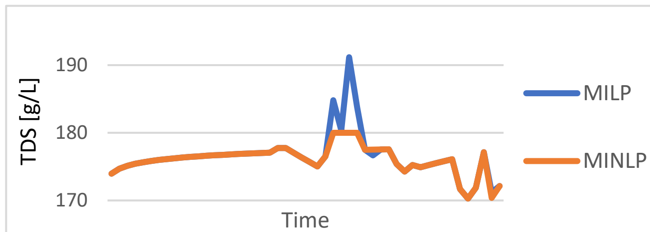

Figure 5. The TDS (g/L) level at a specific location in the PW network.

With both these methodologies in play, a pivotal aspect is the role of water treatment centers. The efficiency of these centers in component removal and water recovery is integral to determining the final quality and quantity of treated and residual streams. The PARETO framework provides flexibility by allowing users to define specific water recovery and removal efficiency targets for each treatment site and technology.

PARETO Treatment and Desalination

Treatment systems are critical in achieving the required water quality for diverse applications such as beneficial reuse and critical minerals recovery. The costs linked to these treatment systems, varying with the purpose and intensity of treatment, play a substantial role in determining the overall investment in PW management strategies. It is, therefore, imperative to give due consideration to the cost and functionality of treatment models within the broader context of produced water management strategies.

PARETO advanced water treatment analysis: PARETO provides three methodologies (high-level cost analysis, semi-rigorous, and rigorous cost analysis):

1) discrete numerical inputs to enable flexible sizing of treatment plants (PARETO documentation includes a detailed literature review and vendor survey of treatment CAPEX and OPEX: https://pareto.readthedocs.io/en/latest/model_library/water_treatment/index.html).

2) the deployment of detailed rigorous models for comprehensive process design and network optimization.

3) the application of surrogate models for streamlined computational analysis.

Notably, while discrete numerical inputs facilitate the estimation of treatment costs, they fall short in capturing the intricate interplay between water quality and cost implications. To bridge this gap, this work presents a PARETO surrogate modeling approach. These surrogate models adeptly establish correlations between water quality, plant capacity (measured as flow rate), and cost, thereby furnishing a more rigorous cost analysis framework.

PARETO effectively leverages the WaterTAP [5] library's rigorous models, which include a selection of advanced desalination technologies. Among these, Osmotically Assisted Reverse Osmosis (OARO), Mechanical Vapor Compression (MVC), and Membrane Distillation (MD) are prominent for their applicability in treating hypersaline produced water. The presented case study includes these technologies alongside primary treatment processes to produce both purified water and clean brine for beneficial reuse and network recycling, respectively.

The methodologies utilized in PARETO, as previously detailed, provide a platform for diverse approaches in water treatment analysis. To showcase and compare these capabilities, we evaluate three distinct cases, each reflecting a different strategy within the PARETO framework:

Case 1: Discrete Input Values: In this approach, the PARETO framework is applied to analyze a system with discrete input values, where cost data for discrete expansion sizes of the plants are provided. The model uses this data to evaluate and identify the most cost-efficient desalination method among Mechanical Vapor Compression (MVC), Membrane Distillation (MD), and Osmotic Assisted Reverse Osmosis (OARO).

Case 2: MILP-NN Surrogate: This approach involves the use of the MILP integrated with a surrogate neural network (NN). Operating under fixed feed quality assumptions typical of Permian produced water with 128,000 mg/L Total Dissolved Solids (TDS), the model allows for variability in feed flow rate, demonstrating the effectiveness of MILP-NN in systems with fixed quality and variable flow rates.

Case 3: MINLP-NN Surrogate: This case employs an MINLP model, incorporating a surrogate for the MVC process. It enables analysis under varying inlet feed quality and flow rate, providing a comprehensive view of the system's performance under different conditions.

Surrogate Models

Surrogate models are essential for simplifying complex processes in situations where computational limitations (i.e., large scale network problems such as produced water networks), lack of algebraic representation, or external functions/constraints are present.

In our study, we address the complexities of Mechanical Vapor Compression (MVC) produced water treatment technology, which features a non-linear, nonconvex nature, making it unsuitable for direct representation in the large-scale Mixed-Integer Linear Programming (MILP) framework. To manage the substantial increase in problem size from the MVC model's 54 constraints/variables (per time period), we employ surrogate models based on simulations and empirical data, focusing on regression techniques.

Machine learning surrogate models, particularly Neural Networks with Rectified Linear Unit (ReLU) activation functions, are integrated into PARETO strategic model optimization frameworks. These models are applied to MVC plant scenarios, focusing on inputs like water quality and recovery, and outputs including CAPEX, OPEX, and energy consumption.

This work leverages the IDAES-PSE [6] machine learning toolset to train surrogate models for the treatment technologies and integrate the surrogate model within the PW network problem to determine the optimal selection of treatment technologies (case 2 and 3 mentioned above).

PW Quality and Treatment Results

The results presented in Table 2 provide a comprehensive overview of the model's performance across the various cases.

The overarching goal here is not to compare these cases on absolute numbers but rather to demonstrate the PARETO framework's flexibility and adaptability. The basis of calculations and underlying assumptions varies for each method, reflecting the diverse scenarios and user requirements each case study aims to address. This framework is designed to cater to a range of user needs, offering tailored solutions for different operational conditions and types of analysis.

An important observation across all cases is the model's effectiveness in optimizing water management, particularly in its emphasis on recycling water for completions purposes. The data shows that a significant portion of produced water, approximately 45%, is recycled, which substantially reduces reliance on freshwater sources (only about 4%).

Table 2: PW quality and treatment results. [a] kbbl

	Case 1	Case 2	Case 3
Total Cost, k$	18,603	18,470	18,306
Sourced Water[a]	515	515	515
Disposal Volume[a]	7,218	7,000	7,100
Reuse Volume[a]	8,805	8,805	8,805
Piping OPEX, k$	15	14	13
Disposal CAPEX, k$	142	140	140
Pipeline CAPEX, k$	111	113	127
R03 treatment tech.	MVC	-	-
R03 inlet salinity, g/l	134	128	130
Run time, seconds	272	400	1600
Gap, %	0	0	13

As shown in Table 2, the model suggests investing in pipeline, treatment, and disposal infrastructure as an optimal long-term solution. This recommendation is based on a detailed cost-benefit analysis, indicating that such investments, despite their initial capital requirements, are beneficial in the long run for sustainable and efficient water management.

Case 1: Basic Approach with Discrete Input Values: Case Study 1 represents a fundamental yet effective approach, utilizing discrete input values for treatment costs and plant sizes. This method simplifies the analysis by not tracking water quality within the network, focusing instead on optimizing cost and size parameters. One of the significant advantages of this approach is its reduced computational intensity. As indicated in the results, this method can solve the network in just 272 seconds, demonstrating its efficiency and suitability for quick assessments or preliminary planning phases.

Another notable aspect of Case 1 is its suitability for scenarios where vendor or industrial data is available in a discrete format. This approach aligns well with situations where the costs and technologies for water treatment are not heavily dependent on the inlet water quality. It is particularly beneficial in cases where the variation in water quality across the network is minimal, allowing for a more straightforward optimization process without the need for intricate quality tracking mechanisms.

Case 2 Advanced Approach with Surrogate Model Integration: Case 2 incorporates a neural network based surrogate model that is responsive to both inlet flowrate and inlet water quality. To maintain the MILP structure while capturing the effects of varying costs associated with plant capacity and treatment, the water quality in this model is assumed to be a fixed value, representative of the conditions in the Permian Basin. A key attribute of Case Study 2 is its ability to strike a balance between computational efficiency and the adaptability of the model (reaching zero gap after 400s).

One of the most notable features of Case 2 is its capacity to effectively capture the nuances of centralized versus decentralized treatment systems. By providing a finer-scale comparison that takes into account varying treatment cost and plant sizes in various location, this model delivers insights crucial for the consideration of transportation costs associated with water movement to the treatment centers.

Further enhancing the model's capabilities, Case 2 can incorporate an iterative procedure yielding to a dynamic and adaptable analysis by leveraging the post-processing approach (i.e., estimate cost/performance, update quality levels, and re-estimate cost/performance, until convergence is reached).

Case 3 - Advanced Modeling with MINLP and Quality Tracking: Case Study 3 employs an advanced MINLP model that intricately incorporates aspects of water quality, flowrate, and recovery. The scope of Case 3 extends beyond mere operational optimization. It is specifically designed to not only address environmental and regulatory considerations, but also efficiently predict treated water, recovery, and concentrated water. Which is critical to enable beneficial reuse (i.e., recovery of critical minerals from produced waters).

While Case Study 3 offers the most detailed and sophisticated analysis among the three models, it is also the most computationally demanding. As evidenced by the results, this model requires a significant amount of time to reach an acceptable optimality gap. This computational intensity reflects the model's complexity and the depth of analysis it provides. Users of Case Study 3 need to be cognizant of the trade-off between its comprehensive analytical capabilities and the time and computational resources required.

QUANTIFYING EMISSIONS AND ENVIRONMENTAL JUSTICE IN PRODUCED WATER NETWORKS

Accurate estimation of emissions is not only critical for maintaining regulatory compliance but also for the economic considerations of PW systems, especially with the introduction of new emissions regulations. The Inflation Reduction Act, for example, established the Methane Emissions Reduction Program which introduces a charge for reported waste emissions beginning in 2024 [7]. While emissions measurements are generally acknowledged, there is also a growing interest in environmental justice impact. In 2021, the Justice40 initiatives in response to Executive Order 14008 outlined new guidance for environmental justice, including specific recommendation for the decrease of environmental exposure and burdens for Disadvantaged Communities. [8].

The PARETO framework includes three categories of environmental impact and environmental justice measures: (1) air pollutant metrics, (2) environmental exposure in disadvantaged communities, and (3) trucking activity. Air emissions are tracked at different sources throughout the system: trucking, pipeline operations, pipeline installation, disposal, storage, and treatment. Five measures of air pollutants were identified for this case study: Greenhouse gas emissions (CO2 equivalents), NH3, NOx, SO2, and $PM_{2.5}$. Table 2 presents the respective coefficients. PARETO reports on air emissions at each source and across the full PW network for each air pollutant type. Total emissions are also calculated as the sum across all pollutant types. To incorporate emissions metrics into PARETO decision-making, users can select to optimize the PW network with an objective to minimize total emissions.

Table 3: Air emission coefficients.

Source	Unit	Type	Coefficient
Trucking	g/hour	CO2	2,035,000
		NH3	35
		NOx	12650
		SO2	770
		PM2.5	121
Pipeline Operations	g/bbl-mile		
		CO2	22
		NH3	0.0002
		NOx	0.014
		SO2	0.0071
		PM2.5	0.00086
Pipeline Installation	g/mile		
		CO2	310,000,000
		NH3	2,800
		NOx	190,000
		SO2	100,000
		PM2.5	12,000
Disposal	g/bbl	CO2	970
		NH3	0.13
		NOx	9.5
		SO2	2.8
		PM2.5	0.87
Storage	g/bbl-week	CO2	1,000
		NH3	0.012
		NOx	2
		SO2	0.65
		PM2.5	0.076

Table 3 and Table 4 present coefficients used to estimate air emissions output for unit of time, volume, distance, or combination, depending on the source. Air emissions coefficients and mathematical constraints are based on environmental impact modeling in Bartholomew & Mauter [7]. Ongoing work for emissions measurement includes establishing coefficients for technologies beyond Mechanical Vapor Compression.

Table 4: Treatment technology air emission coefficients.

Treatment Technology	Type	Coefficient (g/week)
Mechanical Vapor Compression	CO_2	9600
	NH_3	1.45
	NO_x	12.8
	SO_2	13.5
	$PM_{2.5}$	1.5

The second category included in the PARETO framework addresses environmental justice and focuses on Disadvantaged Communities (DAC) as defined by the Climate and Economic Justice Screening Tool [9]. This metric is a function of air emission measures and reports the air pollutants contributed from sources in the produced water system that fall within a DAC. Ongoing work for environmental justice measures includes incorporating penalties for building new PW infrastructure into an environmental objective function.

The third category reports trucking activity for the total volume of water trucked and total hours of trucking time with non-zero water load.

Environmental Impact Assessment

The above-mentioned metrics have been added to the PARETO framework. Figures 6 to 8 present detailed emissions for the given produced water network. The results presented correspond to Case 1 from the previous section (base case – minimize total cost). It is worth noting that, in the context of this case study and based on the specific data analyzed, the emissions originating from disposal, storage, and pipeline operations are minimal compared to those from treatment and pipeline installation. For this reason, they are not depicted in the figures but are instead included in the analysis.

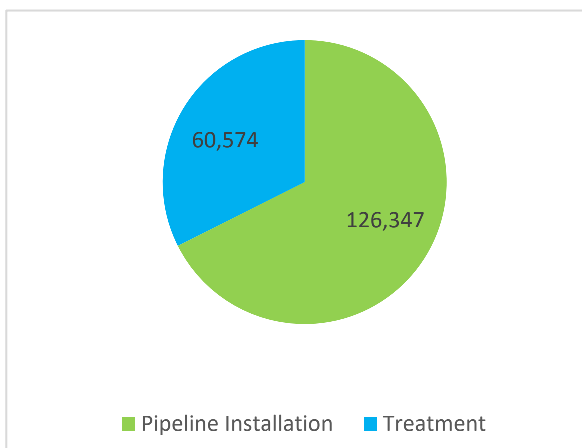

Figure 6: CO_2 emissions in PW networks [kton].

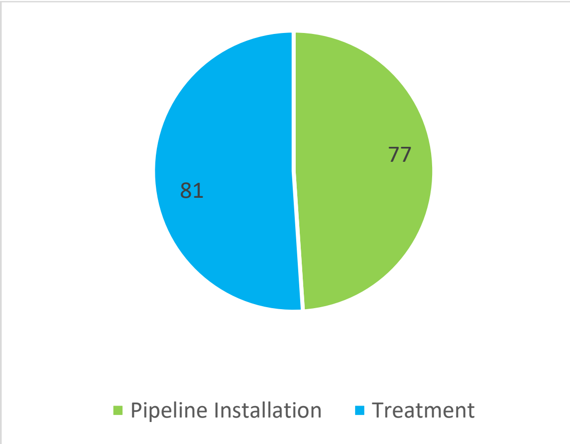

Figure 7. NO_x emissions in PW networks [kton].

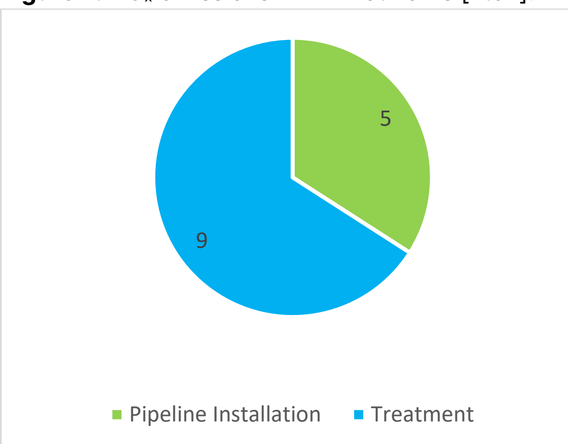

Figure 8. $PM_{2.5}$ emissions in PW Networks [kton].

Emissions Trade-offs in Produced Water Management

The emissions calculations presented in Table 5 of our study provide insightful findings on the environmental tradeoffs of various produced water management strategies. These results reveal the trade-off between minimizing costs and reducing total system emissions. The data indicates that while some strategies effectively reduce overall costs, they may result in higher total emissions. Conversely, approaches focused on minimizing emissions demonstrate a substantial decrease in environmental impact but at an increased cost. These findings underscore the complexities involved in balancing economic and environmental objectives in produced water management, highlighting the need for multi-faceted approaches that consider both financial and ecological sustainability.

For the given case study, PARETO framework reduced PW treatment in favor of increasing produced water disposal to reduce the overall emissions. This result can be seen as contradicting from the water sustainability perspective, presenting a potential opportunity to explore different environmental objectives.

Table 5: Results environmental KPIs.

Objective (minimize)	Cost	Emissions w/ limits
Total Cost (k$)	18,603	20,410
Total Emissions (kton)	126,486	126,482
Sourced Water (kbbl)	515	515
Disposal Volume (kbbl)	7,218	9,312
Reuse Volume (kbbl)	8,805	8,805
Piping operational costs (k$)	15	12
Disposal CAPEX (k$)	142	286
Pipeline CAPEX (k$)	111	127

It is crucial to acknowledge the intrinsic limitations of the network studied, particularly in the context of the Permian case study which primarily relies on piping for water transportation. Piping, as demonstrated by prior research [10], offers emission savings compared to trucking, which is absent in our base case scenario, inherently limiting the scope for further emission reductions. Furthermore, the scope of the presented case study is constrained to a 52-week period, covering only 16 production and completion pads. This limited geographical and temporal scale suggests that the observed emission savings, while seemingly modest, may represent a larger potential for emission reduction across broader basins and over the operational lifetime of wells.

Lastly, it is pertinent to consider that the direct emission savings, while valuable, may not fully capture the broader environmental and health benefits. These benefits are more significantly recognized when emissions are translated into cost dollars in terms of Human Health Effects (HHE). Although the conversion to an HHE-focused objective is beyond the scope of this iteration of the PARETO framework, it represents a critical area for future exploration to comprehensively assess the value of emission reductions.

CONCLUSIONS

This work presents an update on project PARETO's capabilities for advanced treatment modeling and quality tracking, and the quantification of environmental justice and emissions in produced water networks. We demonstrated the use of PARETO framework to determine optimal infrastructure buildout, PW management, and the selection of treatment technologies that will enable potential beneficial reuse options in oil and gas produced water networks.

Further work will focus on demonstrating multi-objective optimization tools for optimizing produced water networks under different objectives (i.e., water quality, cost, emissions and environmental justice, PW reuse, etc.). Additionally, PW quality can be seen as a source of uncertainty in the decision-making process; process design under uncertainty is a promising topic in the area of PW desalination.

ACKNOWLEDGEMENTS

We gratefully acknowledge support from the U.S. Department of Energy, Office of Fossil Energy and Carbon Management, through the Environmentally Prudent Stewardship Program.

Disclaimer: This project was funded by the Department of Energy, National Energy Technology Laboratory an agency of the United States Government, through a support contract. Neither the United States Government nor any agency thereof, nor any of its employees, nor the support contractor, nor any of their employees, makes any warranty, expressor implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

REFERENCES

1. Veil, John. "US produced water volumes and management practices in 2012." Groundwater Protection Council, 2015.
2. L. Capper, "Seismicity and class II SWD Disposal Well Risks. Induced Seismicity: Myth versus Reality and Impacts we can anticipate," AAPG Southwest Section, Midland, Texas, 2017.
3. J. Park, R. Chen, A. Datta-Gupta, S. Lele and T. Tyrrell, "Quantitative Assessment of Induced Seismicity from Hydrocarbon Production and Produced Water Disposal in Azle Area, North Texas," in Unconventional Resources Technology Conference, Houston, Texas, 2021.
4. Drouven, M. G., Calderon, A. J., Zamarripa, M. A., Beattie, K. 2022. PARETO: An Open-Source Produced Water Optimization Framework. Optimization and Engineering. https://doi.org/10.1007/s11081-022-09773-w
5. Beattie, K.S., Gunter, D., Knueven, B., Lee, A., Ladshaw, A., Drouven, M., Bartholomew, T. WaterTAP v1.0.0. Oak Ridge National Lab. (ORNL), Oak Ridge, TN (United States), 2021. [URL: https://doi.org/10.11578/dc.20210527.7]. Lawrence Berkeley National Lab. (LBNL), Berkeley, CA (United States); National Energy Technology Laboratory (NETL), Pittsburgh, PA, Morgantown, WV, and Albany, OR (United States); National Renewable Energy Lab. (NREL), Golden, CO (United States).
6. Lee, A., Ghouse, J. H., Eslick, J. C., Laird, C. D., Siirola, J. D., Zamarripa, M. A., Gunter, D., Shinn, J. H., Dowling, A. W., Bhattacharyya, D., Biegler, L. T., Burgard, A. P., Miller, D. C. 2022. The IDAES process modeling framework and model library – Flexibility for process simulation and optimization. Journal of Advanced Manufacturing and Processing, 3(3), 1-30. https://doi.org/10.1002/amp2.10095
7. Inflation Reduction Act of 2022, Pub. L. No. 117-169, § 60113 (2022), enacting Clean Air Act § 136, to be codified at 42 U.S.C. § 7436.
8. United States, Executive Office of the President [Joseph Biden]. Executive Order 14008: Tackling the Climate Crisis at Home and Abroad. 1 Feb 2021. Federal Register, vol. 86, no. 19, pp. 7619-7633, https://www.govinfo.gov/content/pkg/FR-2021-02-01/pdf/2021-02177.pdf
9. Council on Environmental Quality, https://screeningtool.geoplatform.gov/en/#3/33.47/-97.5
10. Bartholomew, T. V., Mauter, M. S. 2016. Multiobjective optimization model for minimizing cost and environmental impact in shale gas water and wastewater management. ACS Sustainable Chemistry & Engineering 4.7: 3728-3735.

© 2024 by the authors. Licensed to PSEcommunity.org and PSE Press. This is an open access article under the creative commons CC-BY-SA licensing terms. Credit must be given to creator and adaptations must be shared under the same terms. See https://creativecommons.org/licenses/by-sa/4.0/