DECARBONIZING WATER DESALINATION BY OPTIMIZING RENEWABLE ENERGY AND BATTERY STORAGE USING OPTIMIZATION ALGORITHMS

Om Sanan*	Joshua Sperling	David Greene	Ross Greer
Scarsdale High School	NREL		UC – San Diego
11th Grade Student	Researcher	Independent Researcher	Researcher
New York, USA	Colorado, USA	Colorado, USA	California, USA
om.sanan007@gmail.com	joshua.sperling@nrel.gov	dgreenewater@gmail.com	regreer@ucsd.edu

Abstract: The escalating challenges of water scarcity and carbon emissions require a shift towards climate-smart water desalination processes to ensure sustainable management of our water resources. Desalination has significant potential to address water security, yet energy demand and costs are high. This study employs a novel automated Energy Management System (EMS) to accelerate desalination's decarbonization, energy efficiency, and cost-effectiveness using Renewable Energy (RE), battery storage, and Artificial Intelligence (AI). Leveraging Machine Learning (ML) models such as XGBoost and Gradient Boosting, we forecasted water production, energy consumption, and weather based on historical 5-year data from four real life mid-to-large scale U.S. desalination plants. Utilizing sophisticated optimization algorithms such as Particle Swarm Optimization (PSO) we aligned RE generation with plants' energy demands. Results show that our customized innovative ML models accurately forecasted critical variables, achieving normalized Root Mean Square Error of less than 10% for key metrics such as treated water flows, energy demand, temperature, solar irradiance, wind speed, etc. Optimization led to RE system configurations that reduce costs and carbon emissions across all facilities, underpinning the study's objective of fortifying water security for a resilient water supply infrastructure and ensuring sustainable operation of desalination plants amidst climate change. A RE optimization scenario at the Tampa Bay desalination plant, which dynamically selects the optimal RE percentage between 50% and 100%, led to 99% RE mix of Photovoltaic Energy, Wind, and Concentrated Solar Power (without batteries) resulting in a 98% reduction in CO2 emissions and 1% lower cost compared to the utility baseline; whereas a 100% RE optimization scenario (with batteries) led to 40% higher cost compared to the utility due to high cost of battery storage (Note: Tampa Bay plant has the lowest electricity costs among the desalination plants used in our study).

Key Words: water desalination, reverse osmosis, renewable energy, optimization, energy management, decarbonization, weather forecasting, time series forecasting, artificial intelligence.

I. INTRODUCTION

Water and Energy are critical for sustenance of life on Planet Earth; there is an inextricable link between water and energy efficiency, where each resource's stewardship directly influences the availability and sustainability of the other [1]. According to UNU-INWEH, 5.6 billion people (~70% of the world's population) live in countries that are considered water insecure as of 2023 (including the entire population of Africa); and 2 billion people (~26% of the world's population) do not have safe drinking water, a crisis expected to worsen in the coming decades, especially in urban areas [2]. Desalination, especially Reverse Osmosis (RO) has emerged as a viable solution with tested technology to harness vast amounts of seawater and brackish water to produce high quality water, with more than 21,000 operational facilities in 177 countries, increasing at 6.8% annually between 2010 and 2020 [3]. However, it faces two problems: (1) desalination is expensive with energy accounting for 25-40% of the total cost or over 50% of the operating cost [4], and (2) today more than 99% of world's water desalination plants use energy derived from fossil fuels thereby contributing to carbon emissions and climate change.

We present a novel, cost-effective, energy-efficient, and automated Energy Management System (EMS) [5] framework for decarbonizing water desalination by: (1) forecasting water production, energy consumption and long-term weather using ML models based on 10-year hourly historical weather data and 5-year hourly/daily historical operations data from four U.S. desalination plants, (2) integrating with an EMS that uses RE generation and battery storage to displace fossil energy and aligns RE with the anticipated energy demand of these plants, and (3) co-optimizing location-specific RE and battery system sizing and water production schedule to create a resilient water-supply infrastructure capable of navigating sudden changes in environmental conditions and operational demands. Our vision is to replace fossil fuels with RE by 50%-100% for a sustainable future and propose a pathway for energy cost savings.

New water desalination projects in various parts of the world (Spain, Egypt, Saudi Arabia, UAE, Australia and Chile) are integrating desalination with RE. RE technologies are becoming more accessible as a result of technological innovations in continuously improving efficiency and cost. In 2023, the Spanish government authorized a Euro 600 million investment plan for new desalination plants powered by photovoltaic solar [6]. Future desalination plants being considered include power generation from hybrid solar PV, wind power plants and floating PV plants. At the same time, Global Levelized Cost of Electricity (LCOE) of RE has been reducing significantly, per International Renewable Energy Agency (IRENA) from 2010 to 2022 -- PV reduced by 89% to \$0.049/kWh, onshore wind by 69% to \$0.033/kWh, and CSP by 69% to \$0.118/kWh -- in many cases lower than the utility cost [7, 8]. In an effort to diversify its economy away from oil dependence, Saudi Arabia is planning on tapping its abundant solar energy to provide water and sustainable energy needed by its futuristic Neom city. While RE will play an integral part in the decarbonization of water desalination and the electric grid, no single RE source can service the entire need as the RE power source is intermittent [9]. Use of hybrid energy systems and co-optimization of water and energy demand planning, informed by accurate data on RE distribution of a specific geographic location, can lead to substantial cost reductions and enhanced efficiency in resource utilization [10]. Co-optimization of water and energy allows for water to be desalinated based on local electricity production cost, availability of renewable resources, water storage, and battery storage. The complexity of optimal RO-RE design systems, especially coupling hourly electricity operational decisions with long-term investment decision, will require greater use of AI based optimization methods as they tend to be more accurate and provide more efficient solutions [11]. These sophisticated tools offer dynamic optimization capabilities, enabling real-time adjustments to desalination operations based on fluctuating energy availability and demand. Additional strategies that are considered in the optimization include oversizing of RE sources to overcome high battery cost, and varying mix of RE.

II. Related Research

Though several studies have been conducted to optimize the mix of RE and battery storage, existing literature lacks a comprehensive approach to optimize diverse grid-connected RE sources across different regions using real-life RO desalination plants. Additionally, most data utilized in these studies was either simulated or on a small scale.

[12] designed a hybrid RE system coupled with RO desalination using solar and wind energy, battery back-up and multi- criteria AI optimization models. Research conducted at ITC Gran Canarias pilot scale RO units, Canary Islands, Spain, presented a method for the optimal economic sizing of a medium-scale modular seawater reverse osmosis (SWRO) plant powered exclusively by off-grid wind energy and a water storage reservoir that allows coverage to meet freshwater demand without the use of large energy storage devices [13]. [14] incorporated Artificial Neural Networks (ANNs) into the control panel

of a wind-powered SWRO plant to investigate whether the ANNs can manage the feed flow and operating pressure setpoints based on varying electrical power, feedwater conductivity and temperature. [15] demonstrated the potential of ML to forecast solar energy generation and improve utilization in desalination systems. [11] developed a hybrid RE system powered by photovoltaic modules and wind turbines to power a RO desalination plant using PSO – Grey Wolf Optimizer hybrid model to demonstrate the potential of AI for optimizing RE use. [16] explored various ML models including ANNs and Genetic Algorithm (GA) for their effectiveness in RE forecasting by selecting system configurations that optimize cost, freshwater production and energy resource exploitation. [17] conducted a survey for use of ML models for applications in weather and climate forecasting to bridge the gap between short-term and long-term weather forecasting. [18] used statistical methods such as Auto Regressive Integrated Moving Average (ARIMA) for forecasting weather with minimal error.

III. METHODS

This study employs a comprehensive methodology to optimize the integration of RE sources such as Photovoltaic Energy (PV), Wind Power (WT), Concentrated Solar Power (CSP), and Hydro Power (HT) along with battery storage into desalination plants. The methodology encompasses two major components: forecasting and optimization. The forecasting component involves predicting energy demand and environmental conditions that impact RE generation, while the optimization component aims to determine the optimal mix and sizing of RE systems to minimize costs and CO2 emissions. By combining advanced ML models with robust optimization techniques, this approach ensures an efficient, sustainable and cost-effective EMS for water desalination plants. Real-world data from four U.S. mid-to-large water desalination plants (Table 1) is analyzed to optimize RE systems.

Table 1: Data from 4 U.S. Seawater/Brackish Water Desalination Plants [5], [8]

Seawater/Brackish Water Desalination Plants					
	TDS	Water Production		Energy Usage	SEC
Units:	ppm	MGD	m^3 / year	kWh / year	kWh/m^3
Tampa Bay Desalination Plant, FL [1,3]	35,000	8.2	11,288,134	43,023,680	3.81
San Antonio (SAWS), TX [1]	1,325	3.9	5,349,394	5,019,000	0.94
Alameda County Water District, CA [1]	1,111	6.7	9,198,486	4,205,916	0.46
Kay Bailey Hutchison, TX [2]	2,500	9.0	12,433,762	22,380,772	1.80
Total		**27.7**	**38,269,777**	**74,629,368**	**1.95**
Notes: 1) Actual Data from Facilities; 2) Estimated Data; 3) Tampa is seawater, others are brackish					

a. Forecasting Water Production, Energy Demand, and Environmental Conditions

A comprehensive approach was adopted to forecast both energy consumption and water flows, crucial factors in the operation of desalination facilities. A 60:20:20% split was utilized for training, testing, and validation datasets to ensure robust model evaluation while maintaining sample balance. Various models were trained, including SARIMA, Random Forest, and Gradient Boosting Regressors, chosen for their adeptness in handling time series data and capturing intricate patterns. SARIMA, incorporating autoregressive and moving average components, was utilized to address seasonality in data, while Random Forest and Gradient Boosting utilized ensemble techniques to capture complex relationships and achieve superior predictive performance. Hyper-parameter optimization through Grid Search Cross-Validation fine-tuned the models, optimizing parameters such as Number of Estimators, Learning Rate, and Max Depth to minimize error and enhance accuracy.

Furthermore, a sophisticated weather/environmental forecasting system was developed, integrating with Streamlit for interactive data retrieval and visualization. Three forecasting methods, XGBoost, Prophet, and a novel XGBoost average variant, were employed to predict future temperature, Global Horizontal Irradiance (GHI), and wind speed. These models were rigorously validated and optimized, ensuring reliability and accuracy in forecasts. Among the AI models tested, Gradient Boosting and an innovative average method of XGBoost demonstrate the highest accuracy, with normalized RMSE values below 10% for temperature, wind speed, treated water flow, and energy consumption, and approaching 20% for GHI in certain cases [5].

b. Calculation of Energy Generation by RE Sources

The forecasted variables play a crucial role in the optimization process. After forecasting water demand, energy consumption and weather inputs, we input the forecasted weather variables in our RE generation formulas to forecast hourly energy generation by location for each RE source. P_{PV}, P_{csp}, P_w, and P_{hyd} represent energy production from PV solar panels, wind turbines, CSP power towers, and hydro turbines, respectively. The forecasted energy consumption (P_{FC}) serves as the demand that needs to be met by the RE sources and utility power. In the scenario with battery storage, the optimization also considers the state of charge of the batteries. The batteries store excess energy generated during periods of high RE production and discharge it during periods of low production to meet the demand or provide backup power during grid outages, enhancing energy independence and resilience. Electricity can be stored when rates are low and used when rates are high. The constraints on the depth of discharge (DOD) ensure that the batteries are not overused, maintaining their longevity and efficiency. As of April 2023, California eliminated net energy metering, moving towards a net-billing tariff structure, which cut the rate paid to customers for exporting their excess solar production to the grid by ~80%, and has increased battery + solar installation in the state [19].

c. RE CAPEX, OPEX, and Carbon Emissions

We obtained the Capital Expenditure (CAPEX), Fixed Overhead (FOH) and Variable Overhead (VOH) for each RE system from the National Renewable Energy Laboratory (NREL) Annual Technology Baseline (ATB) workbook [20]. We amortized the CAPEX and Fixed Overhead Cost over a 25-year period using a financing interest rate of 5.0% to obtain a fixed monthly payment per unit resulting in fixed annual payment (CAPEX and fixed operating expenses) of $77, $310,206, $77,174, and $126,294 for PV, wind, CSP, and batteries, respectively. High generation production of the RE sources will result in a lower LCOE for the RE system. The CO2 emissions for each utility were sourced from public databases and for each RE system from NREL [21]. Table 2 summarizes our observations and computations.

Table 2: Total Cost and CO2 Emissions for RE and Battery Systems

Per Unit Metrics	Unit Sizing (kW)	CAPEX / kWh	CAPEX / Unit	Rebate %	CAPEX after Rebates / Unit	FOH / Unit	VOH / kWh	Interest Rate	Years	Fixed Monthly Payment per Unit (CAPEX + FOH) for 25 years	Fixed Annual Payment per Unit (CAPEX + FOH) for 25 years
PV	0.7	$1,664	$1,165	20.0%	$932	$12	$0	5.0%	25	6	77
Wind	2500	$1,724	$4,309,398	20.0%	$3,447,518	$68,420	$0	5.0%	25	25,856	310,266
CSP	200	$5,835	$1,167,053	20.0%	$933,642	$11,678	$3	5.0%	25	6,431	77,174
Battery	600	$2,212	$1,327,207	0.0%	$1,327,207	$33,189	$0	5.0%	25	10,524	126,294

	Grid				Lifetime RE / Battery System			
CO2 Emissions	Tampa	SAWS	Alameda	KBH	PV	Wind	CSP	Battery
g/kWh	430	450	450	330	43	13	28	33
g/unit					30	32,500	5,600	19,800

d. Optimization of Renewable Energy Mix

The optimization process in this study aims to determine the optimal sizing and mix of RE sources and battery storage to meet the energy demand of desalination plants while minimizing costs and CO2 emissions. This section outlines the methodology used to achieve these objectives, covering the decision variables, constraints, objective function, and optimization technique. By leveraging the forecasts of energy demand and environmental conditions, optimization ensures a sustainable and cost-effective energy management system for water desalination plants. The optimization process involves balancing the use of PV arrays, wind turbines, CSP units, and hydro turbines, alongside battery storage and utility power. We initially evaluate the following scenarios that illustrate different levels of reliance on RE and battery storage, offering insights into grid independence, cost, and environmental impacts.

The following three scenarios were considered in the optimization process. The scenarios assume no net metering with the utility grid as we wanted to assess the highest level of energy independence.

1. 100% RE with Battery Storage (No Utility): This scenario aims to achieve complete grid independence by only using RE sources and battery storage. The purpose is to demonstrate the feasibility and implications of operating desal plants entirely on RE without relying on the utility grid.
2. 50-100% constraint of RE-mix with Utility (No Batteries): This scenario represents a hybrid approach where a minimum of 50% of the energy demand is met by RE sources, with the remaining demand supplemented by utility power. No battery storage is used in this scenario. It illustrates the transition phase towards higher RE integration while maintaining grid connectivity for reliability
3. 0%-30% RE with Utility (No Batteries): This scenario shows a low reliance on RE, with only 0-30% of the energy demand met by renewables. The utility grid supplies most of the energy demand. This scenario serves as a baseline for comparing the benefits of partial RE adoption.

Defining Decision Variables and Constraints: The decision variables in this optimization problem include the number of units for each RE source: photovoltaic arrays (Npv), wind turbines (Nw), concentrated solar power units (Ncsp), and battery banks (Nbatt). The optimization process must determine the optimal number of each type of unit to minimize the objective function while satisfying all constraints. The following constraints for optimization ensure that the optimized solutions are feasible and practical, maintaining system reliability and longevity:

1. Non-negativity: All decision variables must be non-negative, ensuring a physically meaningful solution: $N_{pv}, N_{csp}, N_w, N_{geo}, N_{batt}, N_{inv}, P_{FC} \geq 0$

2. Renewable Fraction (RF): The RE fraction must be 100%, at least 50%, or at most 30% of the total energy demand in the 3 scenarios: $RF \geq 1, 0.5, or\ RF \leq 0.30$

3. Depth of Discharge (DOD) of Battery Storage: The depth of discharge for battery storage should not exceed 80% to ensure battery longevity: $DOD \leq 0.8$

4. Plant Capacity Limits: The energy produced must be within the capacity limits of the desalination plant: $P_{FC_{min}} \leq P_{FC} \leq P_{FC_{max}}$

Formulating the Objective Function: The objective function is designed to minimize both the cost and the CO2 emissions of the energy system. It is a weighted sum of the total costs and CO2 emissions, where the weights w1 and w2 reflect the relative importance of these two objectives. We have used 50% weightage for each of w1 and w2. The total cost includes CAPEX, FOH and VOH costs for each RE source, with CAPEX being financed at 5% interest cost over a 25-year period. CO2 emissions are calculated based on the lifetime emissions for each energy source; a cost of $50/ton has been assumed for CO2 emissions for Tampa, which represents the federal government Social Cost of Carbon (SCC). Additionally, we ran sensitivity analysis at CO2 emissions cost of $15/ton at the low end, which is the approximate trading level of the RGGI (Regional Greenhouse Gas Initiative) prices, and of $30/ton, which is the approximate mid-point of the aforementioned levels. The objective function can be expressed as:

$$Objective = w_1 \cdot (totalRE\_cost + util\_cost) + w_2 \cdot (totalRE\_CO2\_cost + util\_CO2\_cost)$$

where:

• totalRE_cost is the sum of costs for all RE sources and battery storage.
• util_cost is the cost of any additional energy purchased from the utility grid.
• totalRE_CO2_cost is the cost associated with the CO2 emissions from all RE sources.
• util_CO2_cost is the cost associated with CO2 emissions from utility grid.

The total cost and emissions from each RE source and battery storage are calculated using the following formulas:

$$totalRE\_cost = \sum_{i=1}^{N} (N_i \times FAPU_i + VOH_i \times Energyproduced_i)$$

where, FAPU is the fixed annual payment per unit for each RE and battery system.

$$totalRE\_CO2\_cost = \sum_{i}^{N} (CO2EmissionLifetime/unit_i \times N_i \times \mathrm{CO2CostperTon})$$

Optimization Technique: Particle Swarm Optimization is used to find the optimal configuration of RE units. PSO is a population-based stochastic optimization technique inspired by the social behavior of birds flocking or fish schooling. It is effective for solving complex optimization problems with multiple variables and constraints. In PSO, each particle represents a potential solution (a specific configuration of RE units) and moves through the solution space based on its own experience and the experience of neighboring particles. The movement of each particle is influenced by its best-known position and the best-known positions of its neighbors, updating its velocity and position iteratively to find the optimal solution.

The PSO algorithm can be summarized as follows:

1. Initialization: Generate an initial population of particles with random positions and velocities.
2. Evaluation: Evaluate the objective function for each particle.
3. Update: Update the velocity and position of each particle based on its best-known position and the global best position.
4. Iteration: Repeat the evaluation and update steps until a stopping criterion is met (e.g., a maximum number of iterations or a convergence threshold).

The position of each particle xi is updated according to:

$$v_i(t+1) = \omega v_i(t) + c_1 r_1 (p_i - x_i(t)) + c_2 r_2 (g - x_i(t))$$

$$x_i(t+1) = x_i(t) + v_i(t+1)$$

where:

• vi is the velocity of particle I; ω is the inertia weight.
• c1 and c2 are acceleration coefficients; r1 and r2 are random numbers between 0 and 1.
• pi is the best-known position of particle I; g is the global best position.

IV. RESULTS

On-site RE generation at the desalination plants is optimized not only for location specific weather, RE generation potential, and water demand but also for battery storage and power demand side management. Co-optimization of water and energy using advanced and dynamic ML models is imperative to exploit operating cost savings and minimize carbon emissions while dynamically adjusting for weather changes. It will allow for optimal battery storage and water storage to create a resilient water-supply infrastructure capable of navigating changes in environmental conditions and operational demand. To achieve grid independence and energy security while minimizing cost and carbon emissions, our optimization model recommends a combination of wind, PV, and battery storage at the Tampa Bay plant – the intermittent nature of the RE sources is overcome using a hybrid approach. We assessed hydro power in our analysis, including input variable forecasting, but found the energy generation to be significantly lower than PV, wind, and CSP, and therefore excluded from our final analysis.

The optimization of Scenarios 1, 2 and 3 results in 100%, 99%, and 30% RE mix, respectively based on $50/ton cost of carbon emission for Tampa desalination plant. As shown in Figure 1: Scenario 1 optimization results in 15,838 PV Panels, 18 acres of CSP, 2 Wind Turbines, and 12 batteries, Scenario 2 optimization results in 15,688 PV Panels, 18 acres of CSP, and 2 Wind turbines, whereas Scenario 3 results in 4,036 units of PV Panels, 5 acres of CSP, and 1 Wind Turbine. Figure 2 shows that there is some wasted energy due to assumption of no net metering: Scenarios 1 and 2 have 11% and 15% wasted energy, which results in a higher cost for these scenarios. Figures 3 and 4 show the total cost of all 3 scenarios and the baseline (current 100% utility sourcing) – Fig. 3 shows annual optimization results and Fig. 4 shows optimization results over a 5-year period. Interestingly and coincidently, Scenario 2, 3 and Baseline result in approximately the same total cost of $16.9 million over 5 years (average cost of $3.38 million per year) as the Tampa Bay plant has one of the lowest utility costs in the U.S. at 7.3 cents/kWh, whereas Scenario 1 results in a much higher cost of ~$25 million over 5 years ($5.0 million per year), primarily due to the use of 12 batteries in Scenario 1 to create 100% energy independence. More importantly, Scenarios 1, 2, 3 and Baseline results in CO2 emissions (in grams/kWh) of ~5 million, 1.4 billion, 62.5 billion, and 90.0 billion, respectively, underscoring the significant savings in CO2 by switching to renewables. A 100% RE mix at Tampa Bay can result in CO2 emissions savings over 5-years equivalent to planting 4.1 million trees [22].

Hybrid RE systems are crucial to achieving decarbonization. The CSP systems with power towers and 10-hour storage generate energy by capturing sunlight during the day, converting it to heat, and storing this heat in molten salts. This stored thermal energy can be used to produce electricity at night or during cloudy periods. Hybrid PV-CSP systems combine the immediate electricity generation by PV with the dispatchable electricity of CSP, providing complementary and reliable RE solutions that maximize efficiency and minimize intermittency. Similarly, solar-wind hybrid energy systems complement each other by combining two different weather parameters, especially when it is windy at nighttime or when it is cloudy, thereby reducing intermittency and creating a more stable electricity supply. The use of batteries in Scenario 1 adds to the LCOE but ensures energy independence and protects the desalination plant from wide fluctuation in energy prices. Also, since utility prices tend to increase over time, batteries should be economically beneficial over their useful life. With states such as California eliminating the net metering program, a 100% migration in electric generation from the utility grid to on-site RE generation at desalination plants would lead us to our goal of decarbonization.

Post-Optimization Analysis: After obtaining the optimal configuration of RE units, the results are analyzed to ensure they meet the energy needs and environmental goals of the desalination plants. The total RE production, costs, and CO2 emissions are calculated and compared against the energy demand and capacity limits. The results are aggregated over different time periods (yearly, monthly) to provide a comprehensive summary of the system's performance. Detailed plots and summary statistics are generated to visualize energy production, demand satisfaction, costs, and emissions. These visualizations and statistics help stakeholders understand the performance of the optimized energy system and make informed decisions about sustainable water desalination.

Tampa Bay Desal Plant - Optimization Results (# of Units, Volume, Total Cost)

Fig 1: # of Units by RE Source – Scenarios 1-3

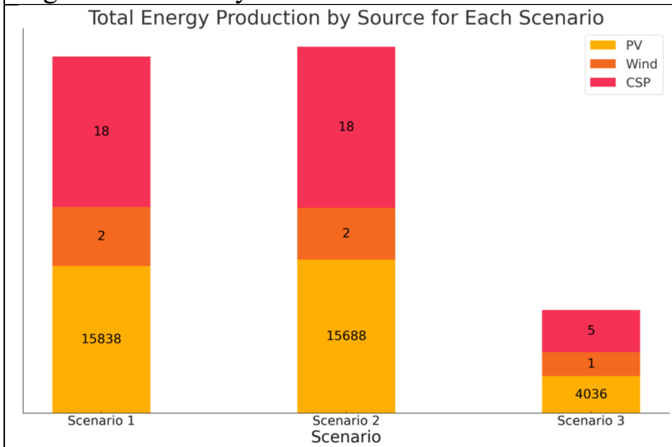


Fig 2: 5-Yr. Energy Gen by Source– Scenarios 1-3

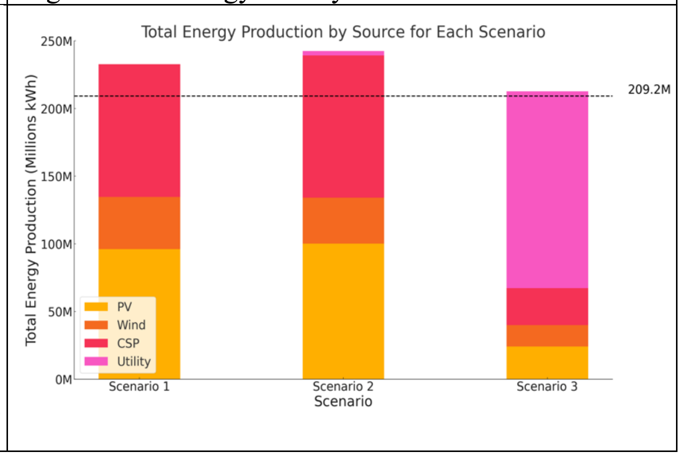


Fig 3: Cost Opt. by Yr.– Scenarios 1-3 & Baseline

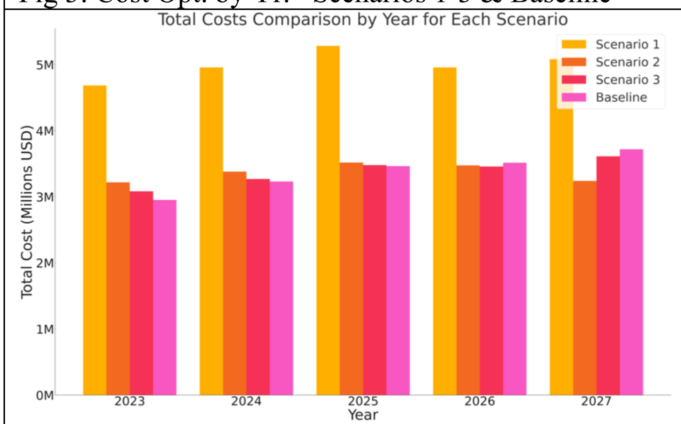
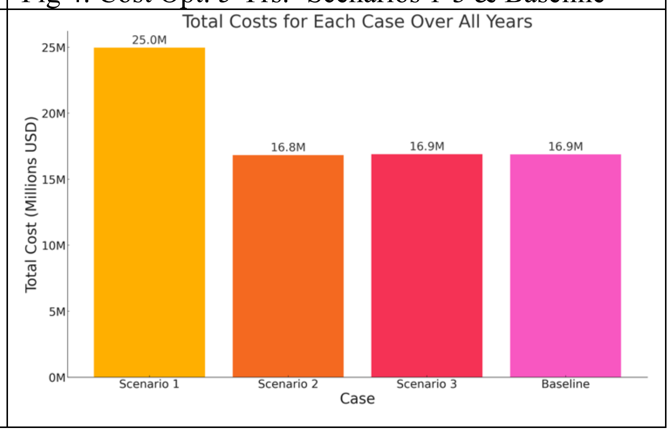


Fig 4: Cost Opt. 5 Yrs.- Scenarios 1-3 & Baseline



V. CONCLUSION AND FUTURE RESEARCH

By integrating advanced forecasting techniques with a robust optimization framework, this study provides a comprehensive approach to designing cost-effective and environmentally sustainable energy systems for water desalination plants. The optimization process ensures that the EMS balances economic and environmental factors while reliably meeting the energy demands of the desalination plants. This holistic approach supports the goal of reducing the carbon footprint of water desalination and promoting the use of RE sources. In the 3 scenarios we evaluated, Scenarios 2 and 3 with RE mix of 30% and 99% (both without batteries) resulted in total cost equivalent to that of the utility baseline, however Scenario 1 with RE mix of 100% (with batteries) resulted in 40% higher cost compared to the utility baseline due to higher cost of battery storage. This goal of onsite RE generation can be extended to other industries.

Future studies can evaluate incorporating demand side management strategies by considering hourly historical and forecasted utility prices, which could mitigate the cost of batteries significantly. Additionally, in the optimization scenarios we assumed no net metering to evaluate a higher degree of energy independence. However, additional sensitivity analysis including net metering could result in further reduction in total cost. Finally, future studies could evaluate the use of geothermal energy and hydrogen storage, water reuse, water and electricity demand reduction, energy efficiency measures, and demand-side management.

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