Load shifting strategies for cost-effective emissions reductions at wastewater facilities

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ABSTRACT

Significant hourly variation in the carbon intensity of electricity supplied to wastewater facilities introduces an opportunity to lower emissions by shifting the timing of their energy demand. This shift could be accomplished by storing wastewater, biogas from sludge digestion, or electricity from onsite biogas generation. However, the lifecycle emissions and cost implications of these options are not clear. We present a multi-objective optimization framework for comparing cost- and emissions-minimizing load shifting strategies at a California case study facility with a relatively low carbon intensity grid and high spread in peak and off-peak electricity prices. We evaluate cost and emissions tradeoffs from optimal flexible operation of both existing infrastructure and optimally sized energy flexibility upgrades. We estimate energy-related emission reductions of up to 9.0% with flexible operation of existing infrastructure and up to 16.8% with optimally sized storage upgrades. Only a fraction of these potential savings is realized under actual industrial energy tariffs and the EPA's recommended social cost of carbon. Energy flexibility may hold promise as a short-term emissions savings solution for the wastewater sector, but the extent of savings is heavily dependent on cost of carbon, electricity tariffs, and emissions intensity of the regional electricity grid.

SYNOPSIS

Quantifying greenhouse gas emissions reductions at wastewater facilities resulting from flexible load operation.

INTRODUCTION

Wastewater facilities account for 1-3% of lifecycle US greenhouse gas (GHG) emissions (**S.1. Wastewater Sector Emissions in the US**), a figure that is expected to increase with more stringent nutrient removal requirements and enhanced demand for water reuse[1]. A wastewater facility's total lifecycle GHG emissions are typically comprised of 22-80% Scope 1[2–7] (i.e., direct gaseous emissions), 4-42% Scope 2[6,8–10] (i.e., emissions from purchased electricity), and 12-65% Scope 3[11–18] (i.e., embodied emissions from manufacturing and biosolids disposal) emissions. Meaningful Scope 1 emissions reduction typically requires a full treatment system overhaul[19,20], which includes substantial capital investment. Scope 2 emissions can be mitigated by generating electricity through biogas combustion[21] or onsite renewables[22], but most facilities purchase electricity from the grid. Scope 3 emissions are outside the direct control of the facility but can be mitigated through supply chain or other operational decisions.

Load flexibility, or the ability of a facility to shift the timing of energy consumption, may offer a cost-effective and rapidly implementable solution for reducing Scope 2 emissions. Since grid emissions vary significantly through the day[6], past work has proposed modulating biological treatment processes[23–25], pumps[26–31], and aerators[27,30,32–34] to reduce load when emissions are high and increase load when emissions are low. One recent case study at a German facility estimates that load shifting could reduce Scope 2 emissions by 5-7% annually.[26] Generally, these prior studies have not fully incorporated the daily, weekly, and seasonable variability of emissions intensity and electricity tariffs. Past work has rarely incorporated the effect of load flexibility interventions on minimizing biogas flaring and associated Scope 1 emissions reductions with cogeneration. Finally, existing studies have underexplored the potential for capital upgrades to wastewater[35], biogas[35], and Li-ion battery[35,36] storage to enhance latent facility flexibility.

In addition to better understanding the potential for load flexibility to reduce Scope 2 emissions, there is significant uncertainty around the impact of load shifting on energy costs. Local electricity tariffs often include both fixed and variable costs that change on hourly and seasonal time scales to reflect the underlying costs of generation and transmission. Peak wastewater treatment demand typically exhibits substantial overlap with peak electricity tariffs, suggesting benefits from shifting demand away from these peaks[28,37–39], but spatial and temporal analysis over several years of operational data is essential to quantitatively evaluating tradeoffs in cost and emissions incentives. High-resolution, site-specific analysis is also critical to the optimal design (e.g., type, size) and operation of storage resources that enhance energy flexibility. In conclusion, the tradeoffs between cost and emissions incentives have not been adequately investigated for long-term operation under electricity tariffs and carbon intensities that vary geographically, seasonally, and hourly.

This paper presents the first comprehensive methodology for analyzing tradeoffs in costs and emissions from flexibly operated wastewater facilities. First, we develop a real-time emissions accounting tool for quantifying the short- and long-term costs and emissions tradeoffs of flexible operation of wastewater facilities. We then formulate a multi-objective optimization problem that solves for the cost- and emissions-optimal operation of a wastewater facility under diverse tariff structures, grid emissions intensities, and assumed social cost of carbon (SCC). We demonstrate our framework by sizing and selecting energy flexibility upgrades at a case study facility.

This framework and subsequent analysis address several critical research questions for the wastewater community. We elucidate the magnitude and variance of wastewater treatment emissions intensity as a function of time and grid mix, as well as degree to which flexible operation of existing facilities can reduce those emissions. Next, we assess the emissions benefits of optimally sized storage infrastructure and elucidate the tradeoffs between cost and lifecycle emissions when designing and operating that storage. Finally, we apply our framework nationally to evaluate the sensitivity of these results to tariff structure, grid mix, and assumed SCC.

METHODS

Scope of Analysis

We summarize the framework's data sources and models in Figure 1. We develop a dynamic emissions model for a wastewater facility that explicitly calculates Scope 1, 2, and 3 emissions and accounts for any changes resulting from storage of raw wastewater, biogas from sludge digestion, or electricity produced by the onsite cogenerator. Scope 1 emissions from biological processes are included in our estimates of total facility emissions but excluded from our dynamic model because of the uncertainty in how emissions might change when storing wastewater for up to 12 hours under well mixed conditions. The impacts of assuming fixed Scope 1 emissions factors are further explored in **S.2.5. Sensitivity Analysis of Historical Case Study Emissions**. The subsequent cost and emissions minimization optimizes the operation of existing and hypothetical storage resources at the facility to identify optimal storage design and operational parameters. Throughout, we account for stochastic variation in facility operation, temporal variation in emissions factors, and mechanisms by which constructing and operating storage resources would change capital and operational costs and emissions at the facility. Finally, we conduct scenario and sensitivity analysis using representative grid emissions profiles, electricity tariffs, fossil natural gas (FNG) tariffs, and assumed SCCs from across the United States.

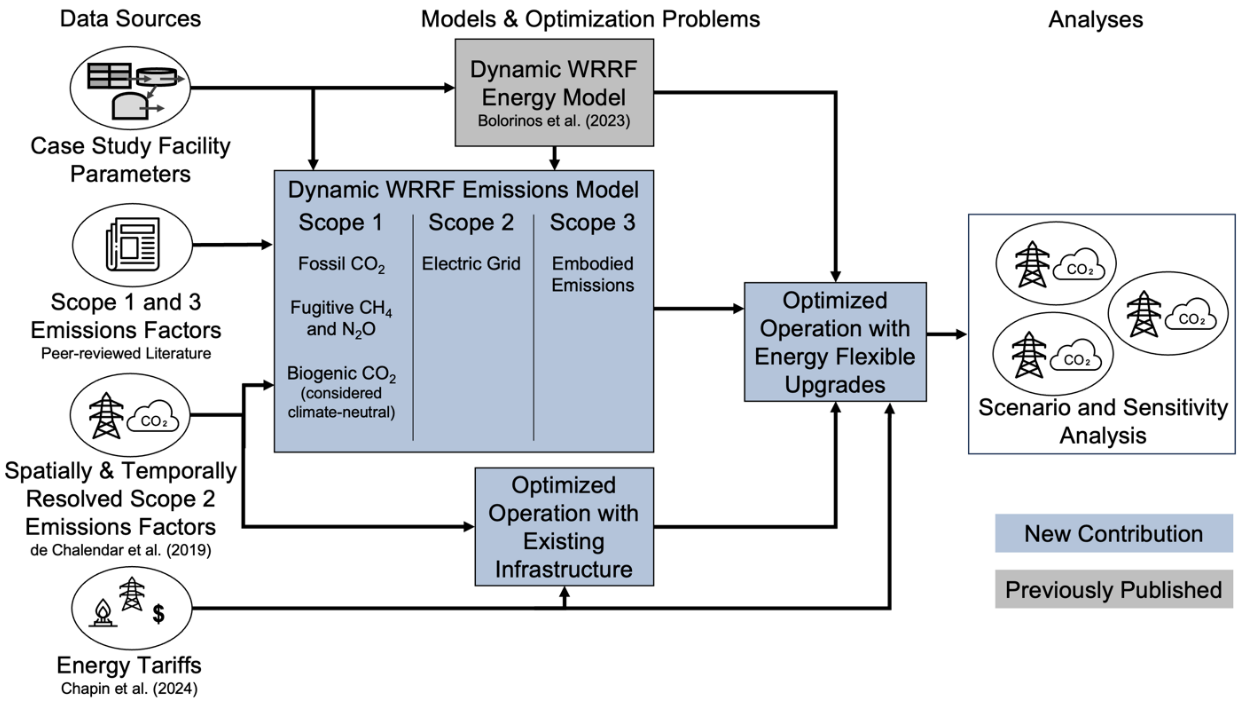

Figure 1. Diagram representing the data sources, models, and outputs of our analysis of wastewater facility energy-related emissions and costs. Energy tariffs are sourced from Chapin et al.[40], grid emissions intensities from de Chalendar et al.[41,42], operational data from our case study facility in California, and literature review of embodied emissions (Supplementary Tables S.3.2, S.3.5, and S.3.6). Bolorinos et al. developed the digital twin and control optimization for cost optimization[35]. We extend that framework to include emissions accounting in a multi-objective optimization problem that balances energy-related costs and emissions.

Dynamic Energy Model

Bolorinos et al. developed a hybrid physics and data-driven model of wastewater energy generation and consumption[35]. Their regularized linear model simulates how storage modulates a facility's gross and net electricity demand and biogas production on a 15-minute timescale, using historical mass and fluid flow data along with hour, weekday, and season covariates to understand temporal trends. We use a 24-hour moving average of mass flow data and 6 lagged samples (1.5

hours on 15-minute intervals) of raw influent wastewater data since the digesters respond more slowly to changes in feed than the primary and secondary treatment trains. We assume that sludge production and resulting biogas production change minimally under the 12-hour maximum retention time constraint for wastewater storage and exclude changes to sludge production from the dynamic model. We select hyperparameters through cross validation that randomly assigned segments to training and test sets.

The Bolorinos et al. model accounts for electricity consumption and generation but does not include heating demand for anaerobic digestion. Operational changes could shift the heat generation from the cogenerator to the boiler and vice versa. Consequently, we extend the Bolorinos et al. model to account for fluctuating heat generation (**S.4.1.1. Heat Demand Constraint**). Under the new heat constraints, we assume that digester heat demand is supplemented by backup natural gas boilers when heat production from the biogas cogenerator is insufficient.

Dynamic Emissions Model

The electricity and heat calculations from the dynamic energy model are inputs into our lifecycle emissions accounting framework. The control optimization focuses on the subset of Scope 1 and 2 emissions directly influenced by flexible operation over the lifetime of an upgrade. We use historical facility operational data both as a baseline for the emissions calculations and to train the dynamic energy model used to simulate operation.

<u>Scope 1 Emissions</u>

Direct gaseous emissions of N_2O, CH_4, and CO_2 are converted to CO_2-eq using their 100-year global warming potential (GWP), though we note that the total emissions are highly sensitive to the GWP time horizon (see **S.2.5. Sensitivity Analysis of Historical Case Study Emissions**). We assume no change to fugitive emission factors from the biological processes within the treatment works due to uncertainty in the magnitude and direction of emissions changes under dynamic operation[2–4] (**S.3.4.1. Scope 1 for Wastewater Storage**). Changes in Scope 1 emissions in our model are limited to changes in volume of FNG combusted in onsite cogeneration and leakage of CH_4 from the biogas holder and cogenerator.

We apply constant emissions factors to the volume of FNG purchased and the volume of wastewater or biogas stored in the problem formulation. Equation 1 computes R_{Scope1}, the reduction in Scope 1 emissions due to flexible operation in ton CO_2-eq. Y_{base} and Y_{opt} are the baseline and optimized FNG combustion timeseries (in m^3), respectively. EI_{FNG} is the emissions intensity of FNG (ton CO_2-eq / m^3).

$$R_{Scope1}(T) = EI_{FNG}[\sum_{t}^{T} Y_{base}(t) - Y_{opt}(t)] \quad (1)$$

We then use Equation S10 to calculate the change in Scope 1 emissions using a functional unit of 1 m^3 wastewater treated. Equation 1 is used with different baselines (Y_{base}) at different stages of the framework.

<u>Scope 2 Emissions</u>

We integrate the facility energy consumption model with electric grid emissions data to calculate the change in Scope 2 emissions resulting from shifting and shedding electricity load. We average grid emissions data from de Chalendar et al. by hour and month during the study period (2018-2020)[41,42] (**S.2.2. Scope 2**). These monthly-hourly averaged emissions factors exhibit less volatility than 15-minute marginal emissions factors and ensure stability when deploying control algorithms[43].

Equation 2 is used to compute R_{Scope2}, the reduction in Scope 2 emissions due to flexible operation in ton CO_2-eq. $EI_{grid}(month_t, hour_t)$ is the average grid emissions intensity (ton CO_2-

eq / kWh) for $hour_t$ during $month_t$. $month_t$ and $hour_t$ are the month the hour at time t, respectively. $X_{base}(t)$ and $X_{opt}(t)$ are the baseline and optimized electric grid purchase timeseries (in kWh), respectively.

$$R_{Scope2}(T) = \sum_t^T [X_{base}(t) - X_{opt}(t)] \times EI_{grid}(month_t, hour_t) \quad (2)$$

We then use Equation S13 to compute the change in Scope 2 emissions using a functional unit of 1 m^3 wastewater treated. Again, different baselines (X_{base}) are used at different stages of the framework.

Scope 3 Emissions

To account for the full lifecycle impact of flexible operation, we incorporate Scope 3 emissions from diverse forms of storage, including raw wastewater storage, biogas storage, and Li-ion battery storage. We estimate the average embodied emissions associated with the manufacturing and construction of energy storage systems through a literature review including national-scale and site-specific examples (Supplementary Tables S.3.2, S.3.5, and S.3.6). Equation S14 uses these emissions factors to calculate $\Delta Scope3_i$, the Scope 3 emissions equivalent per unit of treated wastewater over the lifetime of the upgrade 'i' in ton CO_2-eq / m^3 (**S.3. Added Storage System Emissions Parameters**).

Lifecycle Emissions

We quantify the net change in emissions, ΔE_i (Equation 3), from facilities under various operating schema and upgrade scenarios ('i') in terms of emissions equivalent per unit of treated wastewater [ton CO_2-eq / m^3] by summing the change in emissions from Scope 1, 2 and 3 sources (Equations S10, S13, and S14) over the study period T.

$$\Delta E_i(T) = \Delta Scope1(T) + \Delta Scope2(T) + \Delta Scope3_i \quad (3)$$

Optimized Operation with Existing Infrastructure

We first optimize electricity and FNG consumption (Equation 4) with existing infrastructure based on the market conditions (i.e., grid emissions intensity profile, electricity and FNG tariffs, and SCC). For our case study facility with existing infrastructure, the only optimization variable is the cogenerator's FNG usage. This initial optimization helps to disentangle the operational benefits of upgrades from the altered behavior incentivized by the change in market conditions.

$$minimize \sum_{t}^{T} X(t) \times [E(t) + kEI_{grid}(month_t, hour_t)] + Y(t) \times [G(t) + kEI_{FNG}]$$

s.t. modeling constraints hold (**S.4. Optimization Problem Formulation**) (4)

Where EI_{FNG} and EI_{grid}(month$_t$, hour$_t$) are as defined in Equations 1 and 2, $G(t)$ = FNG cost ($ / m^3), k = SCC ($ / ton CO_2-eq), $E(t)$ = electricity cost ($/kWh), $X(t)$ = electric grid consumption (kWh), and $Y(t)$ = FNG consumption (m^3).

The change in emissions intensity is calculated from timeseries data of historical electricity consumption, X_{hist} as X_{base}; historical FNG consumption, Y_{hist} as Y_{base}; electricity consumption optimized with existing infrastructure, $X_{opt,ex}$ as X_{opt}; and FNG consumption optimized for existing infrastructure, $Y_{opt,ex}$ as Y_{opt}. We plugged $\Delta Scope1$ and $\Delta Scope2$ into Equation 3 with $\Delta Scope3_i$ set to zero when optimizing existing infrastructure.

Optimized Operation with Energy Flexibility Upgrades

We model and optimize the addition of storage to enhance energy flexibility and maximize the reduction in wastewater facility emissions. While we account for Scope 3 emissions implications of storage upgrades, we do not consider other constraints (e.g., footprint) that might limit storage deployment.

We identify cost and emissions-optimal storage types (raw wastewater storage, biogas storage, or battery storage) and sizes for a facility using grid search techniques (**S.5. Grid Search for Optimal Storage Capacity**). The objective function matches Equation 4 with additional mass balance and upper bound constraints (**S.4. Optimization Problem Formulation).** Finally, we use the electricity and FNG consumption time series optimized with energy flexibility upgrades, $X_{opt,up}$ and $Y_{opt,up}$ respectively, to calculate the change in emissions from optimized operation with the upgrade. During sensitivity and scenario analysis, we standardize results in terms of load hour equivalents (LHEs) of storage capacity to ease comparison across diverse forms of energy storage. LHE is calculated using methods detailed in Bolorinos et al.[35].

We differentiate between the cost-optimal and the emissions-optimal operating conditions by setting the SCC, $k = 0$ for the cost-optimized case and setting the energy cost $E(X) = 0$ for the emissions-optimized case. Costs and emissions can be co-optimized by using the true electricity tariff for $\mathrm{E}(X)$ and setting k to the desired SCC. Unless otherwise noted, the cost of carbon used for co-optimization throughout the study is k = $120 ton CO_2-eq.

Case Study Facility Parameters

We demonstrate this workflow for Silicon Valley Clean Water in Redwood City, CA. The case study facility is a publicly owned treatment works serving 200,000 customers with a treatment capacity of 29 million gallons per day (MGD) and an average flow of 13.5 MGD (51.1 megaliters / day)[44]. While the municipality operates a separate stormwater system, it experiences a significant amount of inflow and infiltration, with wet weather peak flows of 2-3 times normal flow. The facility is located in the PG&E service area with the B-20 tariff structure in which there is a time of use charge from 4-9 PM, a concurrent peak hours demand charge of $1.78 / kW during winter and $26.8 / kW during summer, and an all-day demand charge of $20.7 / kW. All demand charges are based on monthly energy demand maxima. The energy model uses 15-minute operational data from September 2018 to December 2020. This data includes metered energy consumption, wastewater volumetric flow, and sludge mass flow rates, biogas production, and heat and electricity generation from a 1.266 MW cogenerator. During the study period, the facility generated 60% of its electricity from biogas. Approximately 10% of biogas was flared due to cogenerator outages and misalignment of electricity demand and biogas production. The optimization framework is adaptable to different facility configurations, as the underlying linear models can be retrained using facility-specific historical data.

Scenario and Sensitivity Analysis

We assess the generalizability of our findings by performing scenario analyses for fixed energy storages sizes of 1 and 2 LHE for each of the three storage types, a total of 12 upgrade scenarios. We also perform sensitivity analysis using electricity and FNG tariffs from the 100 largest wastewater facilities in the US[40] and emissions intensities from 15 different US electric grid areas[41,42]. Finally, we vary the assumed SCC between \$0 and \$525 / metric ton[45] (i.e., k was varied in Equation 4) to inform a marginal cost of carbon analysis (**S.6. Marginal Cost Calculation**). While varying tariff structure and grid emissions profiles, we use a constant SCC of \$120 / ton based on the EPA's recent recommendation[46]. For sensitivity analysis of emissions factors used throughout the model see **S.2.5. Sensitivity Analysis of Historical Case Study Emissions**.

RESULTS

Dynamic Emissions Model

We observe high variance in real-time carbon emissions from our case study facility. This results from variations in wastewater flow rate (Figure 2A), the emissions intensity of the grid (Figure 2B), the price incentive for shifting load to off-peak hours (Figure 2B), and the instantaneous balance between facility energy demand (Figure 2C) and onsite energy generation (Figure 2D). Influent wastewater flow varies from 13,700 m^3 / d (3.62 MGD) to 95,500 m^3 / d (21.7 MGD). The emissions intensity of the California Independent System Operator (CAISO) grid has seasonal and daily variation of up to 100 kg CO_2 / MWh and 125 kg CO_2 / MWh, respectively. In October, the PG&E tariff energy charge is 29.6% higher during peak periods, while the demand charge is 8.6% higher, incentivizing load shifting. Peak hours charges are higher during summer months, and lower during winter months. The emissions and energy profiles are not aligned (e.g., at night the electricity price is lowest, while emissions are highest), so the optimization problem must account for tradeoffs between the two incentive signals.

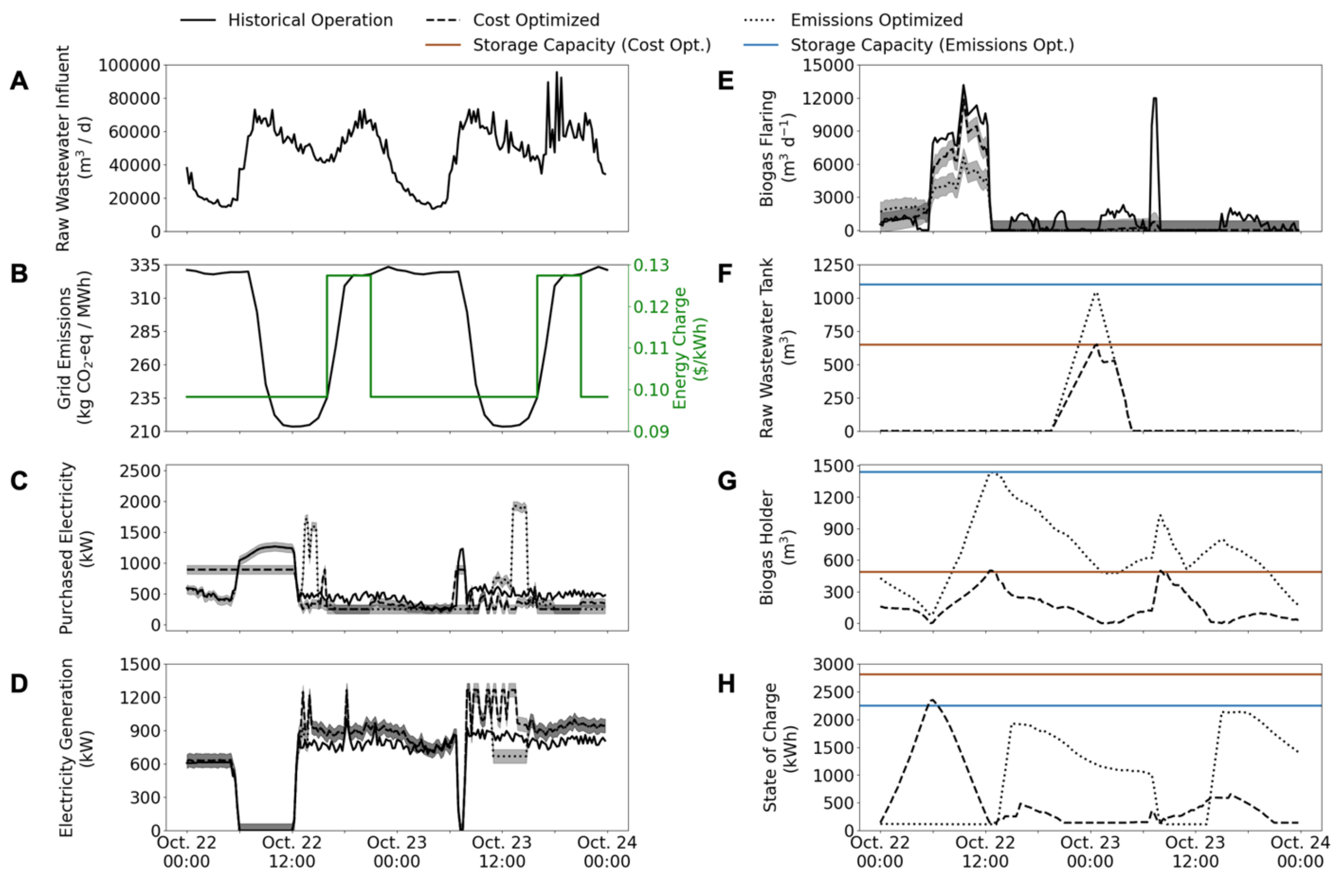

Figure 2. Representative historical time series data and storage-optimized facility operation from October 22nd and 23rd 2019 for our case study facility, Silicon Valley Clean Water. In the historical scenario, the facility has a cogenerator and no raw wastewater (RW), gas holder (GH), or battery (BY) storage capacity. For both the energy bill minimization (dashed line) and emissions minimization scenarios (dotted line), the facility has an equivalently sized cogenerator, but the size

of the RW, GH, and BY storage systems are optimally sized for each scenario. Cost-optimal and emissions-optimal capacities are reported in Figure 3B. The sleeves represent 95% confidence intervals for the optimized simulations. **A)** Historical raw wastewater influent in m^3 / day. **B)** The CAISO average emissions profile for October from 2018-2020 and the 2021 Pacific Gas & Electric (PG&E) energy charge ($/kWh). There is a monthly demand charge of 1.78 $/kW with the same peak hours that is not shown. **C)** Net electricity demand in kW (i.e., grid electricity purchases) at SVCW under historical, cost-optimized, and emissions-optimized operation. **D)** Electricity generation under historical, cost-optimized, and emissions-optimized operation. **E)** Biogas flaring rate in m^3/day under historical, cost-optimized, and emissions-optimized operation. **F)** State of storage for RW in m^3 for emissions-optimized and cost-optimized operation. **G)** State of storage for GH in m^3 for emissions-optimized and cost-optimized operation. **H)** State of storage for RW in kWh for emissions-optimized and cost-optimized operation.

Given this operating environment, we estimate a treatment emissions intensity of 0.75 kg CO_2-eq / m^3 of water treated, for a total of 14 kiloton CO_2-eq / year. Of that annual total, Scope 1 is 7.4 kton CO_2-eq, Scope 2 is 1.0 kton CO_2-eq, and Scope 3 is 5.6 kton CO_2-eq. Approximately 70% of Scope 1 emissions are biological process-related, rather than energy-related (**S.2.4. Historical Case Study Cumulative Emissions**). Scope 2 emissions would be 3% higher if we did not account for the hourly and monthly variation in emissions intensity of the grid. The low Scope 2 baseline emissions for this case study facility stem from 65% of electricity demand being generated via onsite cogeneration, with up to 9% FNG blended with biogas, and the remainder coming from California's relatively low-emissions grid (250 kg CO_2-eq / MWh in CA vs. 375 kg CO_2-eq / MWh national average). As a result, this case study represents a conservative estimate of the emissions impact of flexible operation. Our results focus on changes to *energy-related emissions*, which include Scope 2 emissions and the 30% of Scope 1 emissions related to cogeneration.

Optimized Operation with Existing Infrastructure

The operational objective function has a significant effect on the energy costs and Scope 2 emissions of the case study facility. In the absence of energy flexibility upgrades at the case study facility, optimizing the timing of electricity consumption could reduce energy costs by up to 2.6% (i.e., SCC = \$0 / ton CO_2-eq). An objective function seeking to minimize carbon emissions, without regard for electricity costs (i.e., electricity cost = \$0 / kWh), is expected to reduce facility emissions by 9.0%. This decrease primarily stems from a substitution of electricity sources, namely decreased reliance on electricity generation from FNG and increased electricity purchase from the relatively low emissions intensity CAISO grid.

Optimized Operation with Energy Flexibility Upgrades

Next, we explore the potential for further reductions in cost and emissions intensity achievable through expanded onsite storage of raw wastewater, biogas, and electricity. To facilitate direct comparison between storage technologies, we evaluate the cost and emissions benefits of capacity upgrades for the combination of storage types and each standalone storage type (Figure 3A). For each scenario, we identify the cost-optimal and emissions-optimal storage type and size (Figure 3B). The optimal storage capacity is very sensitive to the objective function, with optimal storage sizes varying by up to an order of magnitude between the emissions and cost-optimal cases.

A two-day period (October 22nd-23rd, 2019) of optimized operation using the optimized combination of storage capacities is shown in Figure 2C-H. On October 22nd, the net electricity demand did not follow the typical diurnal profile peaks in the early afternoon and evening due to a cogenerator outage in the middle of the day (Figure 2D). We intentionally select this abnormal day to visualize the ability of flexible operation to manage fluctuations in biogas generation and demand and reduce flared gas and Scope 1 emissions. Besides a brief cogenerator outage, the facility operation was more typical on October 23rd. When the energy storage capacity and operation of the facility is optimized for costs on a typical day, the net demand is kept flat throughout the day to avoid demand charges (Figure 2C). By contrast, the facility has a large demand peak during minimum emissions hours in the emissions-optimized scenario.

The state of storage in Figures 2F-H highlight the operational differences between the cost- and emissions-optimized scenarios. In the cost-optimized scenario, the battery is charged earlier on October 22nd and discharged during the cogenerator outage to decrease peak demand (Figure 2H). By contrast, the battery in the emissions-optimized scenario is charged later in the day when the emissions intensity of electricity is lower. The timing of raw wastewater storage use is similar across the two scenarios, but the storage utilization is higher in the emissions-optimized scenario (Figure 2F). While both cost-optimal and emissions-optimal operation involve storing biogas during the cogenerator outage to minimize flaring and maximize energy recovery (Figure 2G), biogas flaring is more successfully mitigated in the emissions-optimal scenario due to the larger storage capacity (Figure 2E).

Lifecycle Emissions Tradeoffs from Energy Flexibility Upgrades

We compare the annual average lifecycle emissions impacts of cost-optimal and emissions-optimal design and operation of facilities with expanded energy flexibility in Figure 3A. Cost-optimal operation using existing storage infrastructure increases energy-related emissions by 10.7% (or 7.61 g CO_2-eq / m^3 wastewater treated) compared to historical emissions. When flexibility directly reduces flaring (i.e., the gas holder scenario), the cost-optimal operation also reduces emissions due to an increase in gross onsite electricity generation. In other scenarios, the cost-optimal operation with expanded storage further increases emissions because PG&E electricity tariffs are not aligned with CAISO emissions intensity for this case study facility. For example, cost-optimized operation with a battery reduces Scope 2 but increases Scope 1 emissions by importing FNG to produce lower-cost electricity with the cogenerator. This increase is further exacerbated by Scope 3 emissions of the battery.

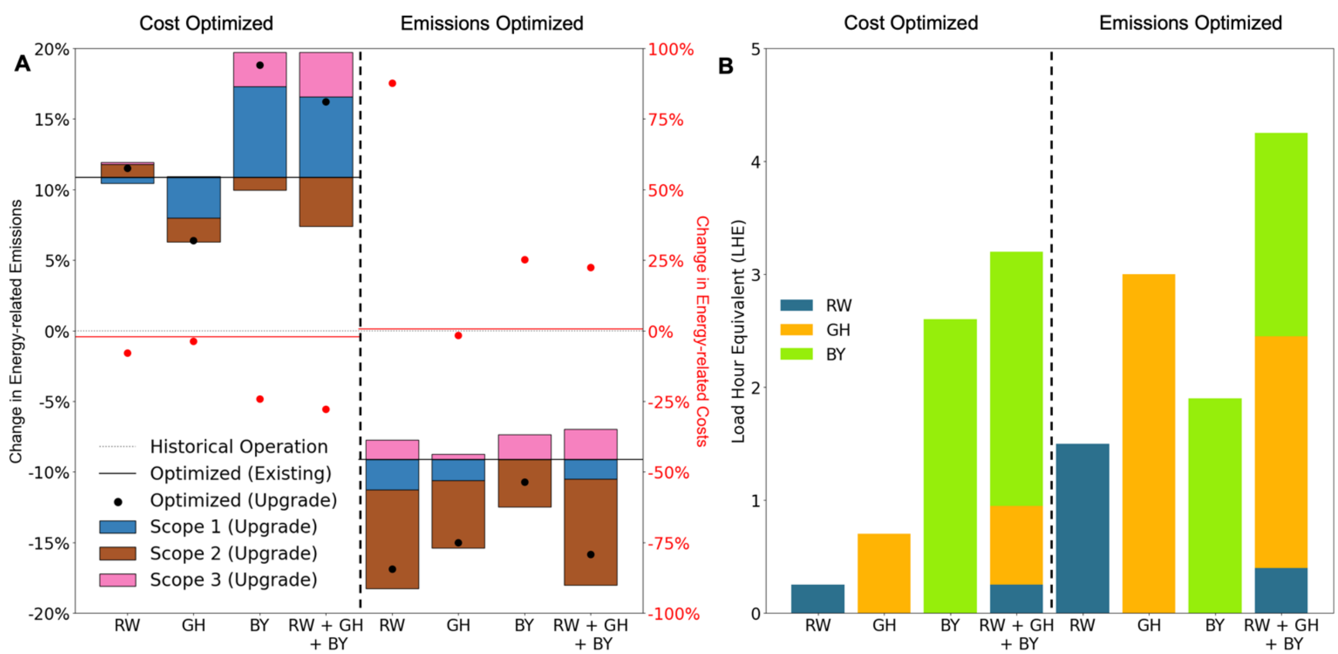

Figure 3. Greenhouse gas emissions changes when deploying and optimizing the use of energy storage for cost and emissions reductions. **A)** Emissions are broken down into direct fugitive emissions from methane leakage and FNG combustion (Scope 1), electric grid emissions (Scope 2), and embodied emissions of the energy flexibility upgrade (Scope 3). Four storage systems are modeled: raw wastewater (RW) storage tank, low-pressure biogas holder (GH), and Li-ion battery (BY), and a combination of the three (RW + GH + BY). For each storage system, two scenarios are considered: cost-optimized (SCC = \$0 / ton CO_2-eq) and emissions-optimized (electricity cost = \$0 / kWh). The cost implications are shown in red. **B)** The optimal storage capacities sized using a grid search in each scenario, with the sizes normalized to load hour equivalents (LHEs).

In contrast to cost-optimized upgrades and operational strategies, emissions-optimized energy flexibility upgrades offer significant additional emissions reduction benefits. Optimized energy flexibility upgrades yield an additional 2-8% energy-related emissions reductions on top of the 9% reduction without infrastructure upgrades. The largest lifecycle emissions decreases are achieved using raw wastewater storage (16.8% or 12.0 g CO_2-eq / m^3 wastewater treated).

In all the emissions-optimized cases, however, the resulting emissions decreases incurred large financial losses from increased energy bills. The emissions-optimal raw wastewater storage scenario incurred an 87.9% increase in the facility's energy bill compared to historical operation. This is equivalent to an average marginal cost of $7,100 / ton CO_2-eq, suggesting a low likelihood of achieving this degree of carbon emissions in practice. A more realistic scenario with a flat tariff and $120 / ton CO_2-eq SCC is investigated in **S.7. Optimization with Flat Tariff**.

Finally, we consider the tradeoffs in cost and emissions intensity using a multi-objective optimization formulation with SCC ranging from $0 to $525 / ton CO_2-eq (Figure 4A). The three storage systems are compared at 1 and 2 LHE capacities (as opposed to the cost- or emissions-optimized capacities from Figures 2 and 3) to fairly compare the impact of optimizing across SCCs. Despite being equivalently sized, the energy flexibility upgrades have different tradeoff curves due to the different ways in which they interact with system dynamics. For example, operating the 2 LHE gas holder under a SCC of $120 / ton CO_2-eq achieves nearly all the reduction that would be achieved at $525 / ton CO_2-eq. Battery operation does not reduce emissions as much at $120 / CO_2-eq, but it has the largest range in its tradeoff curve, indicating that it is more sensitive to the SCC. Flexible operation of raw wastewater storage has the least potential for emissions reduction for the SCCs analyzed, a stark contrast to the 100% emissions-optimized result in Figure 3A, when raw wastewater showed the largest emissions-reduction potential.

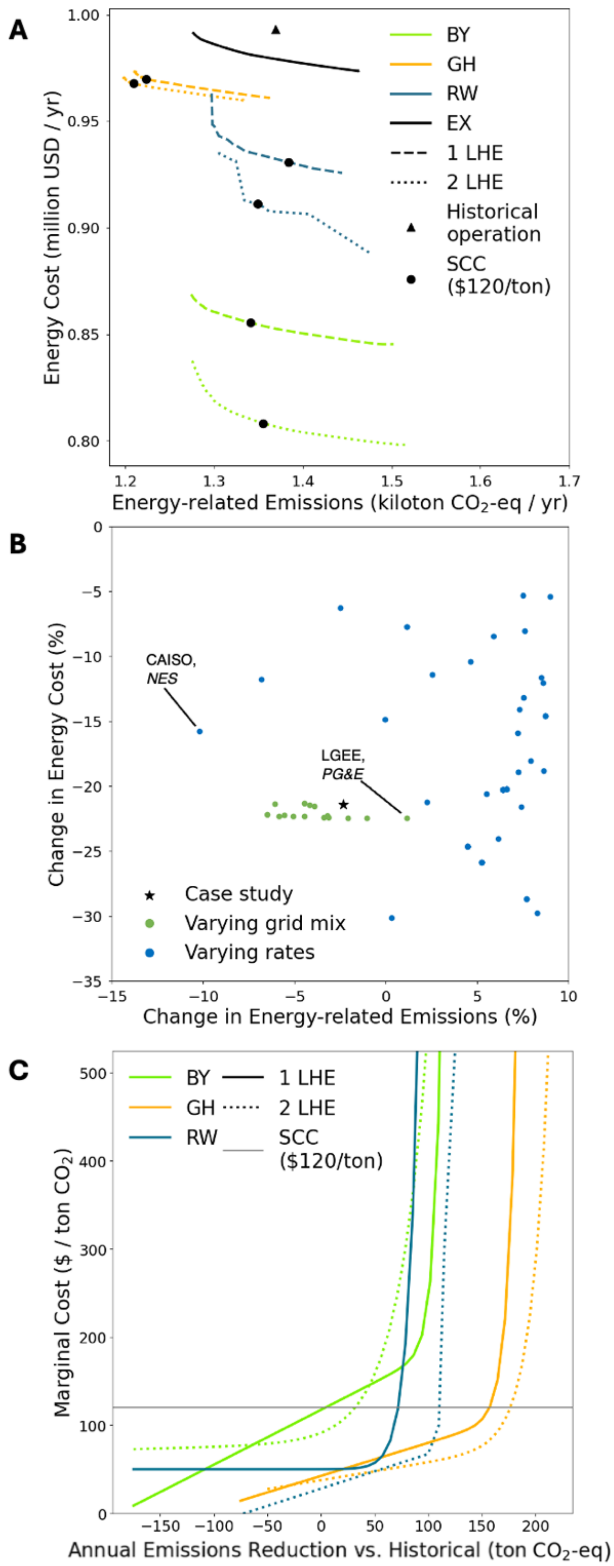
A
B
C
Energy Cost (million USD / yr)
Energy-related Emissions (kiloton CO2-eq / yr)
BY
GH
RW
EX
1 LHE
2 LHE
Historical operation
SCC ($120/ton)
Change in Energy Cost (%)
Change in Energy-related Emissions (%)
CAISO, NES
LGEE, PG&E
Case study
Varying grid mix
Varying rates
Marginal Cost ($ / ton CO2)
Annual Emissions Reduction vs. Historical (ton CO2-eq)
SCC ($120/ton)

Figure 4. Annual energy-related costs and emissions at a wastewater facility under different storage, rate, and grid emissions intensity values. **A)** Tradeoff curve between energy-related emissions and costs resulting from energy flexibility in a wastewater facility in the San Francisco Bay Area. One and two load hour equivalents (LHEs) of different energy storage systems (raw wastewater storage (RW), low-pressure biogas holder (GH), and Li-ion battery (BY)) are compared to optimization of existing infrastructure (EX) under the actual Pacific Gas & Electric (PG&E) rate structure as of November 2021[40]. Each curve represents the results of optimizing both electricity and fossil natural gas (FNG) consumption using a social cost of carbon (SCC) ranging from \$0 to \$525. The points on each curve represent a SCC of \$120 / ton CO_2-eq. The triangle indicates energy-related emissions and costs for historical operation. **B)** The impact of market forces on optimal energy-related emissions and costs is represented as a percentage compared to unoptimized operation examined by (i) simulating the case study facility with a 2 LHE battery under the rate structures for the largest 100 wastewater facilities in the US with a SCC of \$120 / ton CO_2-eq and CAISO emissions intensities, and (ii) simulating the case study facility with a 2 LHE battery, the emissions intensities of 15 different grids across the US, PG&E tariffs, and a \$120 / ton CO_2-eq SCC. The star indicates the optimized operation under the real-life energy tariffs and grid emissions intensity of the case study facility (PG&E and CAISO) with a \$120 / ton CO_2-eq SCC. Two examples are highlighted, Nashville Electric Service (NES) and CAISO from varying tariffs and PG&E and Louisville Gas & Electric and Kentucky Utilities Energy (LGEE) from varying grid mix. **C)** Marginal cost curves for BY, GH, and RW in both 1 and 2 LHE capacities compared to a \$120 / ton CO_2-eq SCC. Due to the fitting procedure, marginal costs are only valid for the domain of the raw data (\$0-\$525 / ton CO_2-eq).

Scenario and Sensitivity Analysis

Given the sensitivity of the facility's optimal emissions to both grid emissions intensity and tariffs, we perform sensitivity analysis by simulating operation in other markets. We apply electricity and FNG tariffs from the 100 largest wastewater facilities with CAISO grid emissions and 15 grid emission profiles across the US with PG&E tariffs with a 2 LHE battery and compare the percent emissions reduction for optimized operation versus unoptimized operation in the same market (Figure 4B). We choose a 2 LHE battery since it has the largest range of emissions in Figure 4A.

When optimizing with a \$120 / ton CO_2-eq SCC there is always a cost reduction versus unoptimized operation. Conversely, there is a wide variation in percent change in energy-related emissions from negative to positive. As seen from the star representing our case study, California is near the median in terms of percent change in energy-related costs and emissions, indicating that some markets have more and some less potential for cost-effective emissions reductions through flexible operation. For example, maintaining the CAISO grid mix but using the Nashville Electric Service (NES) tariff achieves an additional 7.9% emissions reduction (104 tons CO_2-eq/yr) with only 5.6% increase in costs (\$57,000/yr) compared to optimized operation under the PG&E tariff. Optimizing the Louisville Gas & Electric and Kentucky Utilities Energy (LGEE) grid mix with PG&E rates leads to a 3.4% increase in emissions (45 tons CO_2-eq/yr) with virtually no change in costs. For context, the average CAISO power plant has an emissions intensity of 245 kg CO_2-eq / MWh.

Finally, we reformulate the results from the tradeoff curve to examine the average marginal cost of CO_2 reductions between cost-optimal and emissions-optimal operation (Figure 4C). Over the sweep between a SCC of \$0 to \$525 / ton CO_2-eq, the average marginal costs are \$254 / ton CO_2-

eq, \$80 / ton CO_2-eq, and \$102 / ton CO_2-eq for the 1 LHE raw wastewater storage tank, gas holder, and battery, respectively.

DISCUSSION

Wastewater treatment accounts for 75% of air emissions damages from the US water sector for an estimated value of \$1.63 billion in the Clean Watershed Needs Survey from 2012[21,47]. A significant fraction of these emissions are Scope 2 emissions stemming from electricity consumed in facility processes, especially pumping and aeration. While process-based efficiency audits commonly yield Scope 2 emissions reductions at wastewater facilities, the magnitude of these emission reduction benefits is likely to be modest compared to those available through load shifting. Further, we expect the variability in emissions intensity of regional grids across the US and the rest of the world to increase with increasing renewable capacity.

Our reported results for optimizing flexible operation of existing infrastructure are comparable to previous literature. Reifsnyder et al. found potential for up to an 8.5% and 4.5% reduction in operating costs and electricity-related emissions, respectively[29]. Sweetapple et al. found the potential for a 10.0% reduction in electricity-related emissions without increasing operating costs[23]. We find a 2.6% energy bill savings optimizing for costs and 9.0% energy-related emissions reduction optimizing existing cogeneration infrastructure for our specific case study facility.

We find additional opportunity for reducing emissions and operating costs through optimized infrastructure upgrades. Reductions of up to 20.7% in energy costs and 16.8% in energy-related emissions can be achieved at our case study facility in the CAISO/PG&E service areas when the timing of grid electricity purchases are optimized separately. Were our case study facility to be located in the LGEE service area, these emissions savings opportunities grow to between 13.0% (existing infrastructure) and 24.3% (upgraded energy flexibility infrastructure). These reductions are greatly diminished when co-optimizing for both cost and emissions, even when accounting for reasonable SCCs.

Despite the physical potential for carbon savings through energy flexibility, we identify serious financial barriers under PG&E tariff structures and current values for the SCC. Realizing the maximum 16.8% emissions reduction at our case study facility was associated with an 87.9% increase in electricity costs. This tension is a direct result of the misalignment of the electric grid emissions profile and electricity tariffs in the CAISO/PG&E service area, but similar conditions exist whenever there are large spreads in peak and off-peak hours that do not track the emissions intensity of the grid. In service areas where tariffs are flat, and/or there is no demand charge, these tradeoffs would be substantially reduced or eliminated. Where grid electricity is more emissions intensive than combusting FNG onsite, there is the potential for increased FNG imports to reduce facility emissions.

Our multi-objective optimization framework helps facility operators balance GHG emissions reductions and energy costs by leveraging energy storage. Additional work is needed to incorporate other key operational objectives, like treatment reliability or effluent water quality, and include the contributions of both energy flexibility mechanisms and process efficiency from the wastewater treatment process itself (e.g. aeration controls). Scope 2 reductions also offer air quality benefits that could be incorporated into a broader framework for evaluating the benefits of energy flexibility[21,48]. A growing number of cities in the US are developing climate action plans, and energy-flexible operation provides a low-investment option for modest Scope 2 emissions reductions. Digital solutions, such as our optimization framework coupled with reliable automated controls, provide an opportunity for cities to meet those goals with minimal capital upgrades or burden on operators.

ASSOCIATED CONTENT

Supporting Information

This information is available free of charge via the Internet at http://pubs.acs.org.

(S.1.) Wastewater Sector Emissions in the US (S.2.) Existing Facility Emissions Parameters (S.3.) Added Storage System Emissions Parameters (S.4.) Optimization Problem Formulation (S.5.) Grid Search for Optimal Storage Capacity (S.6.) Marginal Cost Calculation (S.7.) Optimization with Flat Tariff (PDF)

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Author Contributions

All authors have given approval to the final version of the manuscript. The contributions of each author are outlined in the following CRediT statement:

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Jose Bolorinos: Conceptualization, Methodology, Software, Writing (review & editing), Supervision

Meagan S. Mauter: Conceptualization, Methodology, Writing (review & editing), Funding Acquisition, Supervision

Notes

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ABBREVIATIONS

GHG, greenhouse gas; LCA, life cycle assessment; FNG, fossil natural gas; SCC, social cost of carbon; LHE, load hour equivalent; MGD, million gallons per day; CAISO, California Independent System Operator; PG&E, Pacific Gas & Electric; NES, Nashville Electric Service.; LGEE, Louisville Gas & Electric and Kentucky Utilities Energy

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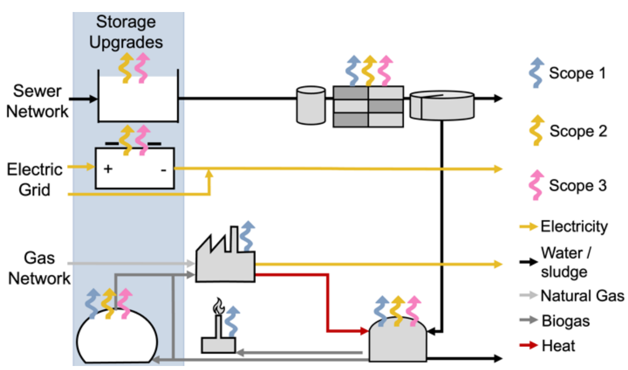

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