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ACCESSING THE RELATIVE SUSTAINABILITY OF POINT-OF-USE WATER DISINFECTION TECHNOLOGIES THROUGH COSTS AND ENVIRONMENTAL IMPACTS

by

BRIGHT ELIJAH

(Under the Direction of Stetson Rowles)

ABSTRACT

According to the World Health Organization, 785 million people lack access to basic drinking water facilities, and 144 million people rely on surface water which is prone to microbial contamination. Pointof-use (POU) water disinfection technologies can be adopted to help address these issues by treating water at the household level; however, navigating various POU disinfection technologies for a given water source or location can be difficult. While numerous conventional POU technologies exist (e.g., boiling water, POU chlorination), new emerging POU technologies (e.g., using novel materials or advanced processes) have been coined by developers to be lower cost with higher treatment capacity. It is unclear if these claims are substantiated and how novel technologies stack up against conventional ones in terms of cost and environmental impacts when considering a necessary level of disinfection for human health. This research compares POU technologies using quantitative sustainable design methods to assess four different POU treatment technologies. The technologies evaluated include chlorination using sodium hypochlorite, silver nanoparticle-enabled ceramic water filter, ultraviolet mercury lamps, and ultraviolet light-emitting diodes. This study leverages open-source Python packages to assess the relative sustainability using techno-economic analysis, life cycle assessment, and disinfection efficacy. Uncertainty is included in all input parameters, and sensitivity analysis (i.e., Spearman's rank correlation) is used to identify which assumptions influence outcomes. The study assumes a household size of 6 people, and a lifecycle of 5 years. Escherichia coli is used as an indicator microbe in characteristic surface and ground waters. We set raw water types to capture the impact of water quality parameters (e.g., turbidity and total organic carbon) on sustainability. Per capita cost (USD·cap⁻¹·yr⁻¹) and global warming

potential (kg $CO_2eq\cdot cap^{-1}\cdot yr^{-1}$) are tracked as sustainability indicators. Study results can potentially inform decision makers, non-profit organizations, and future research on sustainable approaches to safe drinking water through POU technologies.

INDEX WORDS: Water treatment, Disinfection, Point-of-use, Sustainable design, Technoeconomic analysis, Life cycle assessment

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by

BRIGHT ELIJAH

B.S., Benedict College, 2019

M.S., South Carolina State University, 2022

A Thesis Submitted to the Graduate Faculty of Georgia Southern University

in Partial Fulfillment of the Requirements for the Degree

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Major Professor: Committee: Stetson Rowles Francisco Cubas George Fu Jaime Plazas Tuttle

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LIST OF ABBREVIATIONS

Acronyms	Meaning
AgNP CWF	Silver nanoparticle enabled ceramic water filters
CFU	Colony forming unit
EXPOsan	EXPOsition of sanitation and resource recovery systems
GWP	Global warming potential
JMP	Joint Monitoring Program
LCA	Life cycle assessment
LED	Light emitting diodes
NTU	Nephelometric turbidity units
POU	Point-of-use
QSD	Quantitative Sustainable Design
QSDsan	QSD for sanitation and resource recovery systems
SDGs	Sustainable Development Goals
SODIS	Solar water disinfection
TEA	Technoeconomic analysis
UN	United Nations
UNICEF	United Nations International Children's Emergency Fund
WASH	Water, Sanitation and Hygiene
WHO	World Health Organization

CHAPTER 1

OVERVIEW OF THESIS

1.1 Introduction

United Nation's Sustainable Development Goal 6 is centered around universal access to safe and affordable drinking water by 2030, with a focus on the 2.1 billion people that lack access to safely managed water globally.¹ One of the primary issues with poor water quality is microbial contamination which can cause acute health risks, e.g., the spread of diarrheal diseases.^{2,3} To supply safe and potable drinking water, centralized treatment facilities typically remove pathogens through both physical and chemical methods. While such facilities are common in developed countries, centralized systems are costly and require extended construction periods, especially when considering distribution systems.⁴ For example, a new water distribution system in lower income countries is estimated to cost 64-268 USD person⁻¹ for 500-2000 households.⁵ Another study estimated a piped water supply for a small town in Ghana to be 10-14 USD person⁻¹ yr⁻¹.⁶ It is notable that these estimated costs are only for the distribution system and do not include cost for treatment. These barriers make potable piped water out of reach in many developing countries where the need to disinfect water for drinking is urgent. One potential solution for those with microbially compromised water is to disinfect at the household level or point-of-use (POU). POU water disinfection technologies can be a potential pathway for immediate safe drinking water for off-the-grid communities.⁷

Numerous POU disinfection technologies are commercially available, and many more are emerging. These treatment technologies exist over a scale, ranging from conventional technologies (e.g., boiling and POU chlorination) to novel technologies (e.g., ultraviolet disinfection systems).⁸ Typically, researchers investigate the adoption of a unique POU disinfection technology employed as an intervention to microbial contamination of water. For example, solar water disinfection (SODIS) can be a relatively simple intervention for disinfection when properly utilized. A year-long study in Cameroon highlighted that SODIS intervention provided up to a 42.5% reduction in the risk for diarrheal in households that

properly treated their water, but only 45.8% of all households met the determined levels of properly using SODIS after the training.⁹ Ceramic water filters are another POU technology that can be produced with local materials and provide dual mechanisms to remove bacteria, i.e., the porous ceramic matrix and silver nanoparticle coating.¹⁰ A randomized controlled field trial of ceramic filters in Bolivia found them to be effective in meeting World Health Organization (WHO) drinking-water standards even with turbid challenge waters. However, this study was completed over a relatively short five-month period.¹¹ Despite ceramic filters being relatively easy to use, their long-term sustainability has been explored with an agent-based model and can be hindered when the filter maintenance is not completed.¹² Overall, sustained adoption of individual POU technologies can vary between communities due to contextual and end-user factors. Inadequate clarity on how decision makers and stakeholders can navigate the different POU technologies needs to be simultaneously assessed while considering context-specific factors so that engineers, agencies, and researchers can select the most appropriate treatment technology for a given community.

Technoeconomic analysis (TEA) and life cycle assessment (LCA) can be adopted as methods to help evaluate trade-offs in terms of cost and environmental impacts among different POU technologies. These methods are usually leveraged separately to explore either the costs or environmental impacts of different technologies. In one such study, the cost effectiveness was evaluated for POU chlorination (Aquatabs), flocculent disinfection (Procter and Gamble Purifier of Water), and ceramic filters, considering costs related to startup, management, and logistics.¹³ While POU chlorination was found to be the most cost-effective method, this study considered a one year period, which may be shorter than necessary in other contexts. A recent LCA of four ultraviolet (UV) based systems, chlorination, and trucked water delivery found chlorination to have the lowest environmental impacts over various time and scale horizons.¹⁴ Leveraging both TEA and LCA can help identify trade-offs between cost and environmental impacts for POU technologies. These tools together have been used to evaluate technologies (boiling, ceramic filters, bio-sand filters, and POU chlorination). Under a specific set of assumptions, boiling and chlorination had the highest environmental impacts, while boiling was the most expensive (0.053 USD·L⁻¹) and chlorination was the least expensive (0.0005 USD·L⁻¹).¹⁵ Generally, comparing the relative sustainability among different studies can be difficult to accurately complete because assumptions can vary which causes different outcomes for the sustainability indicators. For example, shorter studies with technology lifespans of less than one year may not consider all materials and supplies that are used in the process throughout the technology's lifetime. Assessing the relative sustainability of POU technologies under uncertainty can help to account for the fluctuation in assumptions due to changes over the lifetime, location, and other factors.

The goal of this study is to compare the relative sustainability of several readily available POU disinfection technologies. Specifically, the objectives of this work are to (i) characterize the overall cost and environmental impacts while consider necessary disinfection efficacy of these technologies and (ii) elucidate drivers for sustainability to better inform appropriate adoption in specific contexts. The technologies assessed in this study include: POU chlorination, silver nanoparticle enabled ceramic water filters (AgNP CWF), UV with mercury lamp, and UV with light-emitting diode (LED). This study leverages quantitative sustainable design (QSD) methods for TEA, LCA, and disinfection efficacy assessment. Models and algorithms were developed in several open-source Python packages (QSDsan (QSD for sanitation and resource recovery systems) and EXPOsan (EXPOsition of sanitation and resource recovery systems)).^{16,17} The baseline assumptions of this study were a five year period and six people per household for all systems.¹⁸ Uncertainty was incorporated in the assumption inputted into the models, and sensitivity analysis (via Spearman's rank correlation coefficients) was completed to identify key drivers of sustainability. The impact of context was evaluated by updating assumptions considering two different water compositions. Assumptions relating to technology adoption period were also assessed. Study results can potentially inform decision makers, non-profit organizations, and future research on sustainable approaches to safe drinking water through POU technologies.

1.2 Objectives of Research

This study aims to understand the relative sustainability of four POU technologies and how the technologies will perform in terms of cost and environmental impacts. The objectives of this research include (i) characterizing the overall cost and environmental impacts while consider necessary disinfection efficacy of these technologies and (ii) elucidating drivers for sustainability to better inform appropriate adoption in specific contexts. This comparative analysis employs QSD methods through an object-oriented program in Python to model and analyze the different systems of selected POU technologies. The Python scripts developed in this study can serve as a blueprint for future research to adopt in understanding the sustainability of more novel POU technologies. The relative sustainability of POU technologies can help to guide decision makers in selection and deployment.

1.3 Significance of Study

According to WHO, diseases like diarrhea, cholera, and others caused by microbial contamination have resulted in about 485,000 deaths annually.¹⁹ This contamination comes from people getting their water from untreated and poorly managed sources, e.g., 122 million people use untreated surface water, and about 368 million people use unprotected wells and springs.¹⁹ This study has the potential to contribute towards the successful deployment of POU technologies to improve safe drinking water accessibility at the household level, especially in regions lacking safely managed water. Figure 1 shows the countries of the world in which adoption of POU technologies can be impactful to serve the percentage of the population that lack access to drinking water services. While much of the lack of access to safe drinking is in Africa and Asia, rural or off-the-grid communities in developed counties may also benefit from the adoption of POU disinfection technologies.²⁰ For example, some off-the-grid communities in the United States and Mexico rely on costly bottled water for drinking because their other source is unsafe to drink.^{21–23} The use of POU disinfection technologies may provide cost savings for these communities. Separately, extreme weather events can cause interruptions in piped water supplies and warrant the need for temporary use of POU disinfection technologies while the community rebuilds.

Thus, the potential impact of this study is global as it highlights sustainable approaches to safe drinking water through POU technologies.

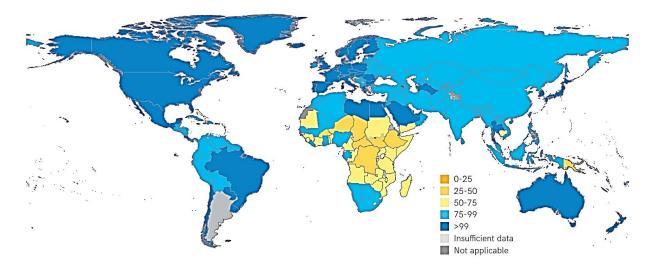


Figure 1. The percentage of population in the countries with access to basic drinking water services. The map is directly from the United Nations.²⁴

CHAPTER 2

LITERATURE REVIEW

A literature review was conducted to gain knowledge of previous research and studies. The literature review covered microbial contamination of drinking water, POU technologies, Short to long term adoption of POU technologies, TEA, LCA, and applications of QSD. Generally, the literature review highlights the lack of access to safe drinking water and the need for affordable and environmentally friendly treatment options for households at a global scale. Numerous studies have been conducted on POU technologies both in the lab and field; however, the sustainability of these technologies remains unclear.

2.1 Microbial contamination of drinking water

Drinking water contamination is not only limited to the water source, as the process of collecting, handling, and storing water can also significantly contribute to increasing microbial contamination.²⁵ The process of treating water at the POU (or household level) and storing treated water before used should leverage practices that avoid recontamination. Many different microbial organisms can be responsible for diseases as a result of consuming contaminated water.²⁶ Some example pathogens include: bacteria (e.g., *E. coli* causing Gastroenteritis), viruses (e.g., *adenoviruses* causing upper respiratory and gastrointestinal illness), and protozoa (e.g., *cryptosporidium* causing Cryptosporidiosis).²⁷ c In this study, we focus on bacterial contamination of water have also adopted *E. coli* as an indicator;^{28–30} due to the fact that the presence of *E. coli* shows the possibility of microbial contamination and can be linked exposure to human or animal fecal pollution from poor sanitation.³¹ It provides a reasonable baseline or indicator for the disinfection efficacy of POU technologies. Although it is notable that some microorganisms are more robust and resistant to certain disinfection technologies.

Another issue that can cause microbial contaminants is the interruption of a treated water supply. Intermittent supply of water is common in some across the globe either based on a set schedule (e.g., water is only available on certain days of the week) or can be due to failures in the supply system. Despite the sources of interruption, it can cause some people to go back to using untreated water directly wherever it may be available. In many cases, use of untreated water can result in health issues that were previously avoided prior to the system failure or breakdown. For example, a community in Uganda experienced an increase in exposure to microbial contamination that was dependent on how long (in days) people had to rely on raw water due to system failure, i.e., the probability of *E. coli* infection increased from 1 in 50,000 people before treated water supply failure 1 in 8 persons after returning to raw water consumption.³² Apart from system failure or breakdowns, any centralized water supply can experience issues that result in health risks to the users. Contamination issues in centralized systems can be linked to an aging system, improper maintenance, inadequate disinfection residual, and infiltration.³³ However, risks to the user in when these issues are prevalent can be potentially prevented with an adequate and proper adaptation of POU technologies. The adoption of POU technologies in communities with a centralized system provides a multi-barrier solution to treatment and can lower health risks. Thus, communities that are vulnerable to such system failures can benefit from our study of informing the sustainable deployment of POU technologies.

2.2 Adopting POU technologies

The need for proper deployment of POU technologies may not be noticeably significant in developed countries (e.g., United States) due to the availability of well-managed centralized water treatment facilities. However, in developing nations around the world, POU disinfection technologies can help to fill an access gap left behind by the lack of adequate centralized water treatment facilities.³⁴ POU technologies also have the potential to be effective in emergency situations like natural disasters, e.g., the earthquake in Haiti in 2010.³⁵ POU technologies can reduce the risk of water related infections if deployed properly with the addition of a proper storage option.^{35,36}

Large scale deployment of the POU technologies with sustained long-term usage remains an issue despite their effectiveness in reducing bacterial infection.³⁷ The effective adoption of POU technologies

requires implementers to manage or keep track of progress to ensure proper and continuous usage. One diarrheal risk intervention study showed that the risk of infection increased with a decrease in the percentage of continuous user compliance in a community.³⁸ For emergency deployments of POU technologies, such as after a flooding event, higher effectiveness has been reported when users are provided with proper training, follow up, and provisions of needed POU materials.³⁹

Another issue associated with the deployment of some POU technologies is sustained adoption by users. After POU technologies are deployed, the initial acceptance and usage has been reported to decline over time, e.g., SODIS and chlorine tablets (Aquatabs) deployed in Flores Island, Indonesia.⁴⁰ Affordability can be a key issue for households when using technologies that require continuous replacement.⁴¹ Sustained adoption as low as 8.1% has been reported in Nigerian communities due to cost of replacement parts and spare parts.⁴² Thus, it is vital for researchers to consider socioeconomic characteristics in a community as well as disinfection efficacy.

For deployment and sustained adoption of POU technologies, it is necessary to understand contextual characteristics like targeted users, geographical context, and water source, as these factors will greatly influence the effectiveness and sustainability.⁴³ It is also essential to compare POU options before deployment in order to deploy the most appropriate option. One such study in Southern African communities evaluated the efficacy of five different POU technologies (i.e., bio-sand filter-standard, bio-sand filter-zeolite, bucket filter, ceramic candle filter, and silver-impregnated porous pot). While this study found that silver-impregnated porous ceramic pot was the most effective and sustainable for the targeted community,⁴⁴ water chemistry also impact the technology performance (i.e., disinfection efficacy). Water quality parameters like turbidity can impact POU technology performance. A specific example is that chlorination has better disinfection efficiency on water with turbidity less than 10 NTU.⁴⁵ It is vital to understand contextual parameters (e.g., local water quality) and how they may influence technology performance and sustainability.

2.3 Short to long term adoption of POU technologies

Increasing numbers of extreme weather events over the last 3 decades (Figure 2) can have a severe impact on water supply and drinking water safety.⁴⁶ In the cases of such events, short term adoption of POU technologies can be help alleviate the issue of lack of access to safely drinking water such events can cause. POU technologies can be deployed in affected areas by response organizations for the people affected to adopt for a short-term period until their water supply is being restored. Adoption of POU technologies for safe water supply in emergency situations is a prominent part of Water, Sanitation and Hygiene (WASH) interventions.⁴⁷ POU technologies can be deployed as a short-term emergency water intervention following a natural disaster if there is access to water source that requires treatment.⁴⁸ It is important to understand which POU technologies can be quickly deployed to such cases in the most cost-effective way while also minimizing the environmental impact of the adoption and disposal of POU technology through the lifetime of usage. More people are likely to use an introduced POU technology in the short period following deployment than in extended period. To ensure extended usage, more monitoring, training and follow up programs are necessary.^{49,50} For cases of disease outbreak linked to water contamination, short term adoption of POU technologies can be a quick preventive measure to deploy.^{51,52}

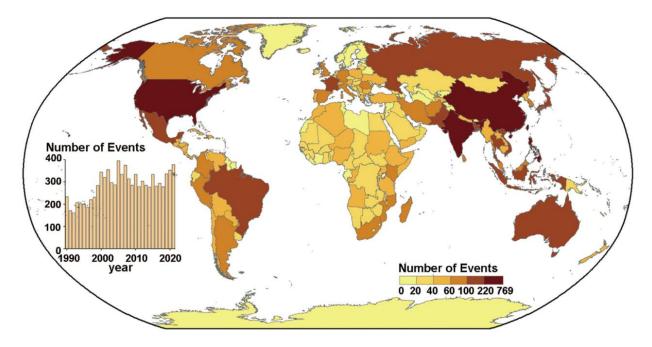


Figure 2: Number of extreme weather events by country or region from 1990 to 2021. These events include mainly storms and floods, droughts, extreme temperatures, and wildfires. Figure is from Wang et al. 2022 with original data from The International Disaster Database.^{46,53}

The United Nations Sustainable Development Goals (SDGs) 6.1 focuses on access to safe and affordable drinking water for all by 2030 which can be measured by the proportion of people with access to safely managed drinking water.¹ Therefore, it is essential to address water safety issues through sustained long-term adoption of POU disinfection technologies in order to improve the progress towards meeting target of the SDGs (Figure 3). The long-term adoption of POU disinfection technologies is not only limited to introducing the technology but also adequate storage vessels in households to prevent recontamination, and the attitude of people towards adoption and usage of POU.⁵⁴ Adoption of POU technologies will be less effective if the usage is discontinued for a period, if the usage is not sustained for an extended period and if people are not fully committed to proper usage. The type of POU technology deployed can also have an impact on sustained long-term adoption of POU technologies over extended

periods of time. For example, the affordability for maintenance and continuous purchase of consumables and spare parts for a technology can impact long-term usage.^{56,57}

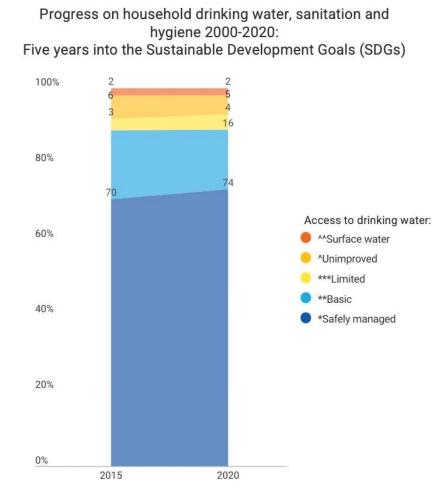


Figure 3: Global progress on household drinking water from 2000 to 2020, i.e., five years into the Sustainable Development Goals (SDGs). Access is broken down into categories of *safely managed (improved source accessible on premises, available when needed and free of contamination),**basic (improved source within 30 minutes round trip collection time), ***limited (improved source over 30 minutes round trip collection time), ^unimproved (an unprotected dug well or unprotected spring), and ^^surface water (drinking water directly from a river, dam, lake, pond, stream, canal or irrigation canal).²⁴

POU technologies has the potential to provide safely managed drinking water to households.⁵⁸ The service level for household drinking water services according to the WHO and UNICEF Joint Monitoring Program (JMP) has 5 categories which are safely managed, basic, limited, unimproved and no service water.^{59,60} The safely managed drinking water is water that is available to users from improved source

without contamination (e.g., fecal contamination). Basic drinking water is gotten from an improved source that requires less than 30 minutes to collect. Limited drinking water is gotten from an improved source that requires more than 30 minutes to collect. Unimproved drinking water is water collected from an unimproved source like unprotected wells and spring. The last category is no service drinking water which is water gotten without treatment from sources like rivers, lake, and ponds.⁶⁰

2.4 TEA of POU technologies

Understanding and capturing the capital and operating costs of technologies are essential to guide selection and deployment.^{61,62} TEA is a methodology that is used to understand the financial viability of a system or technology. This tool that can be used to determine cost as either an absolute analysis of one technology or a comparative analysis to see how various technologies compare to each other in terms of cost.⁶³ This tool has been used in numerous studies on both conventional and advanced POU technologies. For example, TEA was used to access the cost of a novel electrochemical advanced oxidation product POU device in comparison with a commercially available carbon block POU treatment device.⁶⁴ Proper accounting of the capital expenses helped to reveal the cost advantage of the novel POU technologies and the specific parameters that were major drivers for cost.⁶⁴

While many studies have completed cost analysis on POU technologies, most only consider simplified assumptions and are not a full TEA. Some of these studies provide simple comparisons of the capital costs of different POU systems. One such study found chlorination, SODIS, and ceramic filter to be less expensive options compared to coagulation/chlorine system and bio-sand filter by mostly listing only approximate unit costs.⁵⁶ While this work gives a relative idea of cost comparison, but it can be less effective method compared to a complete TEA method as some cost factors are not fully analyzed that can impact both capital and operational expenses.

2.5 LCA of POU technologies

LCA is a methodology that can be used to estimate environmental and human health impacts over a technology's lifetime. This tool that can be used as an comparative assessment of different technologies in an effort to understand how they stack up against each other in terms of environmental impacts over their lifespans.⁶⁵ Similar to TEA, LCA can be used for either an absolute or comparative analysis. Environmental impact indicators (e.g., global warming, acidification, eutrophication, ozone depletion, and ecotoxicity) are used for LCA.¹⁴ These different indicators serve as a guide help eliminate the environmental sustainability of technologies.^{15,66} With LCA, the impact of all individual materials that make up the technology are being taken into account. Apart from the comparison between technologies, these tools can be used to explore what components in each technology are driving change in environmental impacts through sensitivity analysis.

Global warming potential (GWP) is used as a measure of the carbon dioxide (CO₂) emission equivalent to technology's greenhouse gas emission. With CO₂ as the reference gas, GWP lets us understand the relationship between the energy emitted by a ton of gas absorbed over time and a ton of CO₂. GWP is a commonly used indicator of the environmental impacts of technologies used in LCA reports.^{67,68} This indicator can be normalized to yield an understanding of the per capita impact for each person using a selected POU technology covering capital materials and operational components of the technology.

2.6 Application of QSD

QSD methodology enables us to evaluate the relative sustainability of technologies, considering their respective technological components, contextual parameters, and to understand and evaluate key indicators of interest driving change in sustainability (Figure 4).⁶⁹ This methodology leverages tools like TEA and LCA to help inform technology selection, explore the impacts of design considerations, and optimize operational parameters.⁷⁰ QSD has been used to track indicators (e.g., per capita cost and environmental impacts) of technologies for various decision variables, technological parameters, and

contextual parameters.⁷¹ Decision variables are independent parameters that can be adjusted or manipulated by either designers or operators.⁶⁹ Technological parameters are intrinsically defined by the materials and design of a system or technology (are not able to be controlled through design or operation).⁶⁹ Contextual parameters account for the broader conditions in which a system or technologies exists.⁶⁹ QSD framework allows us to track indicators over the simulation space or various combinations of the decision variables, technological parameters, and contextual parameters.

An important feature of QSD methodology is the incorporation of uncertainty. Adding uncertainty to the datasets allows us to accommodate fluctuation in the data set due to factors like time and location. The distribution of uncertainty can follow any form (e.g., triangular, uniform, normal, etc.) or a set to constant in cases where uncertainty is not required like a set volume of container. Therefore, when we run the simulation, it will consider the different possibilities within the range of uncertainty for each data point. Then, sensitivity analysis is performed to understand the key drivers of change in the tracked indicators (e.g., cost and environmental impacts) of the technologies. Therefore, through sensitivity analysis we understand how the change in certain input parameters impacts the changes in the cost and environmental impact of the technology.⁷² This study adopts and leverages QSD methodology for comparative analysis of POU technologies.

Studies have adopted QSD methodology and used it to successfully explore the sustainability of other technologies and design through TEA, LCA and performance.⁷³ For example, QSD has been used to explore and compare the sustainability of designs of non-sewered fecal sludge system for cost and environmental impacts. Through the QSD method, better informed decisions could be made by incorporating environmental impacts. In one is for large scale sanitation systems, lower environmental impacts and higher cost were observed from source separated excreta due to resource recovery compared to treatment of mixed excreta. Thus, decision making for technology deployment needs to consider multiple indicators for more sustainable solutions. QSD methodology also provides a platform to access other factors driving the cost and environmental impacts of the technologies e.g., location related

factors.⁷¹ Another non sewered sanitation system simulated through QSD method was the NEWgenerator systems that the sustainability was accessed through cost and environmental impact with location (i.e., five countries) factored into the simulation to capture the impact of location based factor. In addition to understanding the finance and environmental impacts of the system, the exploring the influence of location on indicators can also achieved through QSD methodology.⁷³

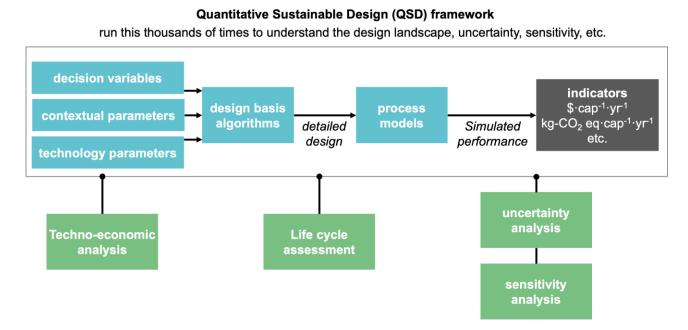


Figure 4: Overview of the quantitative sustainable design (QSD) framework that integrates technoeconomic analysis (TEA), life cycle assessment (LCA), and performance modeling under uncertainty. This figure is based on those presented by Li et al. 2022.⁷²

QSDsan is an open-source Python package that was used to build, model, and run the QSD methods. The QSDsan package uses object oriented programming to perform the QSD operations by simulating the technology systems, allocating cost and impacts of construction materials, developing models and algorithms, simulation, and performing TEA and LCA.⁷⁰ The QSDsan package can be adopted and used to build and evaluate the relative sustainability of different technologies and the documentation, tutorials, and sample python scripts can be accessed online for free. The QSDsan packages allows the user to create components like materials with assigned attributes (e.g., NaOCl),

create the unit systems for the design and simulation of each technology, and develop integrated multiunit systems to simulate performance and complete TEA and LCA of the all the technologies.⁷⁰

CHAPTER 3

METHODOLOGY

3.1 POU technologies

To explore trade-offs among POU technologies, we set parameters based on the design, materials, energy requirements, capital requirements, and operation and maintenance requirements. All essential decision variables and technological parameters were incorporated into the study design based on published research, manufacturers' specifications, and guideline reports. We utilized QSDsan and EXPOsan packages through object-oriented programming in Python to explore trade-offs with TEA and LCA.⁷⁰ All the Python scripts are open-source published on GitHub and have been included in the Appendix.¹⁶ We set general assumptions of a 5 yr study period and 6 people per household for all the POU technologies. The number of people per household is aligned with to the average number of households in most of the countries with lower access to basic drinking water.^{18,24} Raw water quality with varying parameters like turbidity and hardness were modelled with an aim to capture how the systems respond to different water quality sources, e.g., surface versus ground water. We modelled and set water quality parameters for two raw waters (Appendix Table A 5).

The QSD methodology follows the steps in Figure 5 beginning with selecting the POU technologies to be modelled and analyzed. After selecting the POU technologies, we had to build the datasets needed for all the technologies for all components necessary for LCA and TEA. The Python code or script for each POU technology was developed to portray the real-life operation of the technology considering design of technology, construction, and cost using adequate conditional statements, algorithms, constraints, and data. The script for raw water (or influent water) was also developed to reflect the conditions of the raw water quality. The scripts for each technology were compiled and evaluated through the systems for TEA and LCA. The next step included developing the model and analysis scripts which are to run each POU technology system scripts to obtain simulation results which

reflect the uncertainty incorporated in all the inputs. In the final stage, sensitivity analysis was conducted to elucidate which input parameters in each POU technology system influence the indicators.

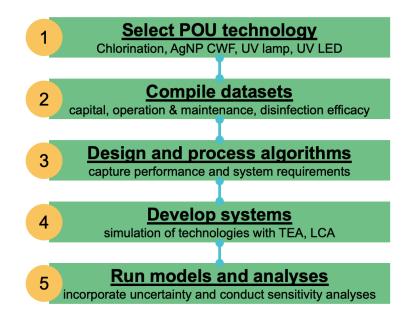


Figure 5. QSD methodology leveraged to develop the models for this work by selecting POU technologies, compiling datasets, developing design and process algorithms, developing systems, and running models and analyses.

3.1.1 POU chlorination. The disinfection method for POU chlorination was designed based on the use of a solution of sodium hypochlorite (NaOCl). This solution is used to disinfect drinking water in households with a simple set up as presented in (Figure 6). The specific NaOCl product used here is marketed as WaterGuard, and each bottle contains 150 mL of the NaOCl solution.⁷⁴ The treated water volume was 20 L based on the assumed container capacity. This disinfection method is designed to be relatively simple to use, where the bottle cover of the WaterGuard bottle is used to dose the NaOCl solution into 20 L of raw water. An expected one WaterGuard bottle cover is a measure of a single dose of NaOCL solution while two is used for a double dose. The full materials and cost inventory data for POU chlorination system is in Appendix Table A 1. The code of this system was designed for three influence streams, i.e., the raw water, NaOCl (chlorine stream), and polyethylene (WaterGuard bottles). The dosing of NaOCl was single dose of 1.88 mg·L⁻¹ at low turbidity (≤ 10 NTU), and at higher turbidity

(> 10 NTU), a double dosed of 3.75 mg·L⁻¹ was used.⁴⁴ Algorithms were developed to capture the impact of water quality, e.g., turbidity on disinfection and potential impact on cost and environmental impacts.

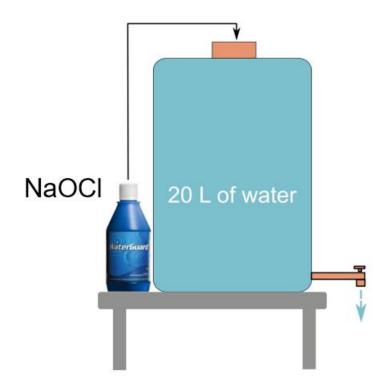


Figure 6. Visual representation of POU chlorination using NaOCl from WaterGuard. This set-up is designed to be easy to use as the cap of the WaterGuard bottle is used to dose the NaOCl solution to 20 L of water for disinfection.

3.1.2 AgNPs CWF. The CWF is coated with AgNPs such that the ceramic matrix filters the water with some bacteria removed while the AgNPs performs the chemical disinfection.⁶⁶ As shown in Figure 7 the setup has the ceramic coated with AgNP placed over a plastic bucket that holds the filtered and treated water. The construction items in Appendix Table A 2 (i.e., sawdust, clay, wood, and polyethylene for the plastic container) were incorporated to account for their costs and environmental impacts.¹⁰ AgNP has been developed in cost through cost effective and eco-friendly methods and made available for water disinfection.^{75,76} The unit has one influent stream of raw water and an effluent of treated water. Here, AgNP is the main consumable as recoating will be needed after every 0.5 to 2 years. The length of time

before recoating the filter with AgNPs varied based on the quality of the water type. Duration of the lifetime for AgNPs in this unit depends on the water quality (i.e., turbidity and hardness). More frequent recoating is expected for higher turbidity and hardness because these constituents have been reported remove more AgNPs.⁷⁷ In this analysis, algorithms were developed to account for the recounting of AgNPs with turbidity > 10 NTU and hardness > 60 mg CaCO₃·L⁻¹.

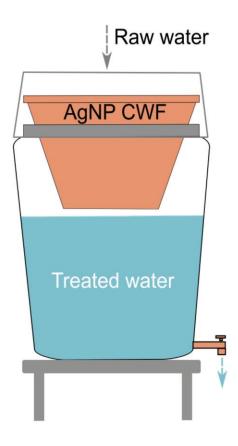


Figure 7. Visual representation of silver nanoparticle-enabled ceramic water filters (AgNP CWF).¹⁰ These point-of-use (POU) disinfection technology have dual mechanisms to remove microorganisms through filtration and chemical disinfection. They are commonly produced with local clays near target communities.

3.1.3 UV with mercury lamp. Low pressure UV lamps were used to design another POU disinfection unit. UV radiation is used to inactivate bacteria when exposed to an adequate UV dose, and the wavelength for disinfection is between 200 to 280 nm.⁴⁴ The system in this study has two UV lamps on opposite sides with water flowing through a quartz tube to maximize light transmittance to microbes as illustrated in

Figure 8. Some of the materials accounted for included quartz, aluminum, polyethylene, and polyvinyl chloride (Appendix Table A 3).⁷⁸ The mercury UV lamps have a lifespan of 2,000 hours set for this studies and varying lifespan has been reported by manufacturers and other studies with some up to 10,000 hours.⁷⁹ The unit is modelled to have two mercury lamps that use 30 W of electricity each. It is designed based on a flow of 9.46 L·min⁻¹ with a UV dose of 215 mJ/mc².⁷⁸ In this unit, we incorporated the impact of water quality through turbidity on UV light transmittance, UV dose, and detention time. This factor influences the energy requirements and potential cost and environmental impacts. The UV lamp was assumed to be on for double the time in higher turbidity > 10 NTU to account for the increased retention time in water with less UV light transmittance. The extended residence time was also accounted for in the unit's electricity demand.

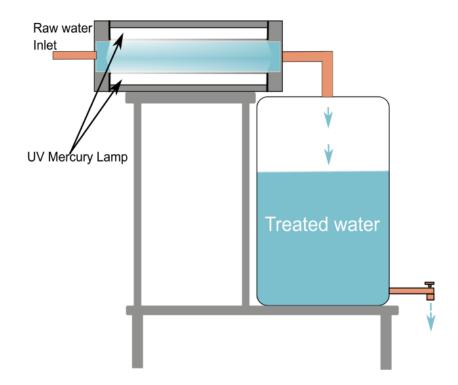


Figure 8. Visual representation of UV disinfection with mercury lamps. This set-up has water that flows through the UV system with two mercury lamps as the source of UV transmission for disinfection. Treated water is then stored in a container for use as needed.

3.1.4 UV with LED. The last POU technology in this study is UV with LED as the source of disinfection. This lights are which are considered more environmentally sustainable as they do not contain mercury like the lamps for traditional UV systems do.⁷⁹ This unit also allows the UV dose to be adjusted and offers design flexibility as the UV LEDs can be arranged in different format to achieve better disinfection. The design capital materials included quartz, stainless steel, aluminum, and 30 UV LEDs. The unit was designed to allow water flow through it in such a way that it is surrounded by arrays of UV LEDs separated from the water by a quartz material that allows adequate transmittance of UV lights for disinfection. As shown in Figure 9 plan view UV LEDs are set up with 15 on each side of the unit.⁸⁰ The system is set up such that an array of UV LEDs require 23 W of electricity.⁸¹ UV LEDs have a life span of 10,000 hours. Other study and manufacturers have reported higher lifetime of up to 100,000 hours although not certain given that the UV LED is still in a developing stage.⁷⁹ The data for the UV LED system is shown in Appendix Table A 4. The unit is designed to incorporate the influence of water quality similar to the unit for UV with mercury lamp. Turbidity of over 10 NTU was assigned a double retention time factor, which also impacted electricity demand.

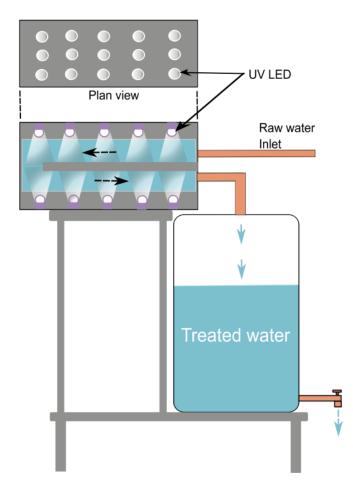


Figure 9. Visual representation of the UV disinfection with LEDs. This set-up has water that flows through an array of 30 UV LEDs with 15 LEDs on each side to allow adequate UV transmission for disinfection.

3.2 Economic analysis

TEA was leveraged to assess the economic requirements of each POU technology. We accounted for capital, operation and maintenance, and energy costs. Discounted cash flow analysis was applied to account for future value of money over the technology's lifespan with a 5% adjusted discount rate on average.⁸² Capital cost covered all the purchases that the units required at start while operation and maintenance accounted for cost estimates of all consumables materials and parts that require periodic replacements. Energy cost requirements were accounted for depending on the electricity need of each unit. It is notable that this requirement does not apply to units without electricity use. The steps for TEA are outlined in Figure 10. The first few steps are to identifying the objective of what cost is to be accounted for, the components of the technology, and factors that contributes to cost (e.g., cost of UV lamp, labor cost). The next step is to compile the data for cost of each material and how often that cost will be applicable for cases of replaceable parts. It is important to note that capital costs are also spread out through the analysis period (5 years in the baseline for this study). The next step is to identify capital cost (construction) and operation and maintenance cost requirement throughout the lifetime of the analysis. We then account for impact of decision variables through design equations and algorithms all units (e.g., dose of NaOCl impact on cost).⁷⁰ The cost analysis was designed to account for impacts of water quality from each unit while achieving necessary disinfection efficacy.

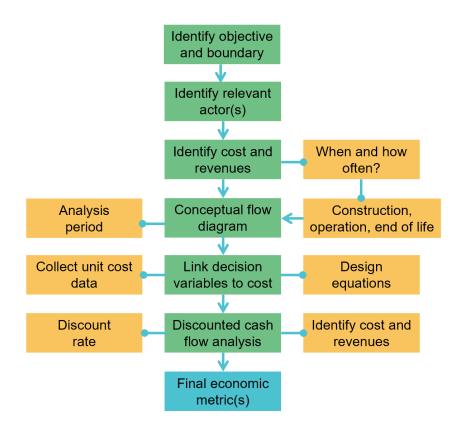


Figure 10: Flowchart showing the steps for the TEA framework for detailed economic analysis through QSDsan.⁷⁰

3.3 Environmental analysis

This work utilized LCA to access the environmental impact of all the POU technologies. This covered impacts from capital impacts, operation and maintenance, and energy requirements. Impact data was obtained from EcoInvent v3.9 database for all the materials and consumables in each unit. Impact data was based on the U.S. EPA's TRACI (Tool for the Reduction and Assessment of Chemicals and Other Environmental Impacts).⁸³ The environmental impacts accounted for global warming potential. GWP is used as a measure of the carbon dioxide (CO₂) emission equivalent to technology's greenhouse gas emission. With CO₂ as the reference gas, GWP lets us understand the relationship between the energy emitted by a ton of gas absorbed over time and a ton of CO2.

The steps for LCA in this study are shown in Figure 11. These steps include first setting the goal and scope. For our analysis, the goal is to track the environmental impacts of capital as well as operation and maintenance requirements of the POU technologies. The inventory analysis is used to account for all the materials and their respective weight (kg) (e.g., weight of NaOCl) and other parameters (e.g., units of UV lamps) in each POU system.⁷⁰ Impact assessment for all the identified parameters and materials to incorporate their respective GWP values based on the data from ecoinvent.⁸⁴ The impact items data obtained from ecoinvent with the corresponding uncertainties are reported in Appendix Table A 6.

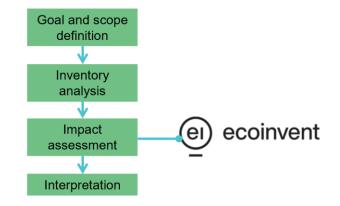


Figure 11: Flowchart showing the steps for performing LCA detailed environmental impacts analysis through QSDsan.

3.4 Water quality and disinfection efficacy

To factor in the effect of water quality, surface water and ground water were modelled based on parameters and assumptions derived from literature. The indicator microbe to access contamination level was *E. coli*. The algorithms aimed to achieve similar log reduction and disinfection efficacy for all systems (i.e., 3 log removal).⁵⁶ To achieve the set level of efficacy for each system, we accessed the required capital materials and consumables based on raw water quality which in turn influences cost and environmental impacts. Therefore, the different water quality parameters for groundwater and surface water sources serve as the contextual parameters modelled into the systems. For example, groundwater source will most likely have hardness due to water dissolves minerals as it moves through rocks.⁸⁵ Both waters have 150,000 – 250,000 CFU/mL of *E. coli*.¹⁰ Note the value for CFU/mL of *E. coli* can vary. Water 1 (a characteristic groundwater) had a turbidity of 1 - 10 NTU and hardness of 60 - 120 mg/L as CaCO₃. Water 2 (a characteristic surface water) had a turbidity of 10 - 30 NTU and hardness of 0 - 60 mg/L as CaCO₃.⁸⁶

3.5 Uncertainty and sensitivity analyses

Uncertainty was incorporated into all assumptions and data for each parameter by adding a variability of 5-25% depending on the data availability and level of confidence. The incorporated uncertainties capture variation in the values for all the data points, e.g., fluctuation in materials cost and impacts. We executed uncertainty through 10,000 Monte Carlo simulations.⁸⁷ Sensitivity analysis was performed to determine factors and parameters that are key drivers to changes in system's cost and environmental impacts. Specifically, we used the Spearman's rank correlation coefficients to measure and analyze the sensitivity of individual parameters for all units.⁷² The report of the Spearman's rank coefficients ranges from -1 and 1, where the values towards -1 have a higher negative correlation and a positive correlation towards 1 (Figure 12). Here, we report the absolute value for the top five Spearman's rank correlation coefficients (> [0.05]) for total cost and GWP for each technology in each water. The

sensitivity analysis can serve as a feedback loop to the QSD framework as it allows developers to identify key parameters and assumptions can be changed or adjusted to access how it impacts results.

Formula for Spearman's rank correlation coefficient:

$$r_s = 1 - \frac{6\sum d^2}{n(n^2 - 1)}$$

Where: $r_s =$ Spearman's rank correlation, d = difference in ranks, and n = number of data points.

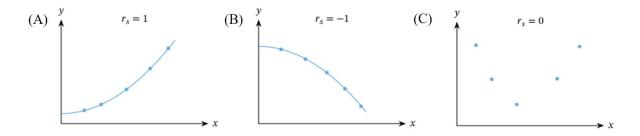


Figure 12: Illustration of Spearman's rank correlation showing (A) a positive correlation, (B) negative correlation, (C) a case with no Spearman's rank correlation.⁸⁸

3.6 Impact of technology adoption lifetime

The baseline assumption was that each technology was used for 5 years. In the next layer of analysis, the impact of the POU technology adoption lifetime was evaluated to determine how the cost and environmental impact of technologies vary from short to long-term adoption. Depending on the context, these technologies may be deployed for a relatively short period (e.g., after extreme weather events cause interruption of a centralize water supply) or a longer period (e.g., as a primary treatment method in underserved communities). The performance of each technology was simulated by setting the use period to 1, 2, 5, 10, and 15 years. Design and process algorithms for each technology were designed to account for the change in the use period to obtain the net cost and net GWP for the different length of adoption.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Economic and environmental sustainability of POU technologies in varying water quality

Since the objective of this study is to characterize the sustainability of readily available POU technologies, this analysis focused on how water quality may impact cost and environmental impacts. The results are reported for all four POU technologies for both water 1 (a characteristic groundwater) and water 2 (a characteristic surface water) in (Figure 13). It is notable that this analysis focused on GWP exclusively for the LCA since it is a high priority of global sustainability indicatives and has been identified as a significant impact indicator in other studies.^{15,89}

4.1.1 Techno-economic analysis. The economic analysis conducted was done to compare the cost effectiveness of deploying each POU technology. The annual per capita cost of each technology is reported and separated to capture capital expenses and operational and maintenance expenses as shown in Figure 13 a, and b. These costs are reported for each technology for water type 1 and 2.

The net cost for water type 1 (a characteristic groundwater) for all four POU technologies is reported starting with the lowest net cost for AgNP CWF system having a net cost of 0.49 USD·cap⁻¹·yr⁻¹ as median and a 5th and 95th percentile of 0.43, and 0.55, respectively (Appendix Table A 7). Henceforth, the percentiles are reported in brackets after the median for all net values. The next lowest cost was POU chlorination with a net cost of 1.34 [0.96 - 1.86] USD·cap⁻¹·yr⁻¹. POU UV (mercury lamp) had a net cost of 3.6 [2.88 - 4.44] USD·cap⁻¹·yr⁻¹, and the highest net cost was for UV LED which was 9.45 [7.35 -11.57] USD·cap⁻¹·yr⁻¹. The low cost for AgNP CWF can be attributed to the low cost of capital materials and production along with low-cost requirements for operation and maintenance. The only consumable for AgNP CWFs is the AgNP recoating which is not as frequent compared to the POU chlorine can be attributed to the simple materials like 20 L jerrycan and WaterGuard (NaOCl) bottle which cost 0.08 to 0.33 USD per bottle.⁹⁰ On the other hand, UV mercury lamp and UV LED require more expensive materials as well as electricity to disinfection water. Comparing the two UV systems, LEDs are more expensive than the mercury lamps, although the lifetime of LEDs are higher with lower electricity requirements.

For water type 2 (a characteristic surface water) (Appendix Table A 8), the net cost followed the same order from lowest to highest; however, the specific cost estimates were higher for water type 2. Net cost for water type 2 starting from lowest to highest were AgNP CWF (0.49 [0.43 - 0.55] USD cap⁻¹ yr⁻¹ ¹), POU chlorination (2.63 [1.85 - 3.65] USD cap⁻¹·yr⁻¹), POU UV mercury lamp (3.76 [2.99 - 4.56] USD·cap⁻¹·yr⁻¹), and UV LED (9.47 [7.38 – 11.60] USD·cap⁻¹·yr⁻¹). The higher operation and maintenance cost associated with water type 2 is due to the need of replaceable parts or consumables. These estimates were significantly higher for chlorination and only marginally higher for AgNP CWFs. Specifically, water 2 required a higher dose of NaOCl for POU chlorination as a double dose of NaOCl is required for higher turbidity.⁷⁴ For the AgNP CWFs, the lifespan of the AgNP coating was lower for water type 2 also due to the turbidity more readily removing the coating and decreasing the lifespan. A lower lifespan resulted in more frequent recoating of AgNP. It is notable that the increase in cost for the AgNP CWFs was only marginal; where the operation and maintenance cost increased from 0.007 to 0.01 USD cap⁻¹ yr⁻¹ from water 1 to water 2, respectively. The turbidity in water 2 required an increase in the electricity run time for POU UV mercury lamps and UV LEDs. This increased run time to ensure proper disinfection increased electricity costs and resulted in more frequent replacement of the lamps. Although the impacts of these additional costs were minimal to the overall costs of the UV mercury lamps and UV LEDs. The higher operation and maintenance cost cause the net cost of deploying the POU technologies to be higher when treating raw water with similar water quality characteristics to water 1 than that of water 2.

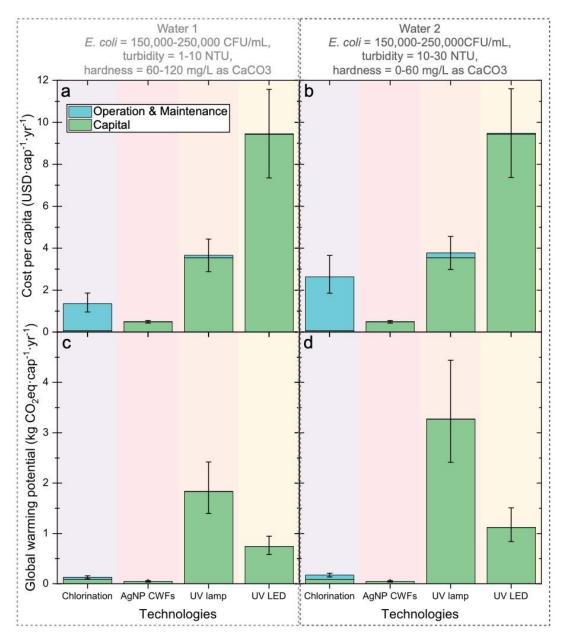


Figure 13. Estimated cost and environmental impacts of POU technologies. The cost USD cap⁻¹·yr⁻¹ for (a) water type 1, and (b) water type 2 for all POU technologies. The GWP kg CO_2 eq cap⁻¹·yr⁻¹ for (c) water type 1 and (d) water type 2. The plots show the cost and environmental impacts on the ordinate and the POU technologies on the abscissa. The overall cost and GWP are broken down into capital as well as operation and maintenance. The median net values are plotted with the error bars representing the 5th and 95th percentile.

4.1.2 Life cycle assessment. For the environmental impacts of each technology, GWP in kg CO₂ eq cap

¹·yr⁻¹ was the environmental indicator used. Environmental analysis through LCA was conducted for all

four POU technologies and for water type 1 and 2 to also access the influence of water quality (Figure 13

c, and d). For water type 1, the lowest overall GWP is AgNP CWF estimated to be 0.046 [0.033 - 0.062] kg CO₂ eq·cap⁻¹·yr⁻¹ followed by POU chlorination at 0.13 [0.098 - 0.16] kg CO₂ eq·cap⁻¹·yr⁻¹. Next greatest was the UV LED with estimated GWP of 0.74 [0.58 - 0.94] kg CO₂ eq·cap⁻¹·yr⁻¹, and the highest GWP was estimated for UV mercury lamp at 1.83 [1.39 - 2.42] kg CO₂ eq·cap⁻¹·yr⁻¹. The GWP was separated for both capital (Appendix Table A 7) (e.g., construction materials) and operation and maintenance (e.g., direct emissions from stream items and consumables). For both UV systems, the capital materials had more impact on GWP than the operation and maintenance, which was mostly electricity and lamp replacement. However, POU chlorination system was also impacted by operation and maintenance due to the need for consumable NaOC1.

For water type 2 (Appendix Table A 8) the estimated GWP from lowest to highest are AgNP CWF (0.046 [0.034 - 0.063] kg CO₂ eq·cap⁻¹·yr⁻¹), POU chlorination (0.17 [0.14 - 0.21] kg CO₂ eq·cap⁻¹·yr⁻¹), UV LED (1.12 [0.84 - 1.51] kg CO₂ eq·cap⁻¹·yr⁻¹), and UV mercury lamp (3.27 [2.41 - 4.44] kg CO₂ eq·cap⁻¹·yr⁻¹). The estimates of GWP followed similar order of lowest to highest impact for both water types. However, due to the impact of water quality on materials requirements (e.g., dose of NaOCl, AgNP recoating, and lamp lifetime), the GWP of water type 2 was relatively higher for all POU technologies than that of water type 1. These results follow the same trends as described for the TEA of water type 2.

Overall, the cost and environmental impacts of these POU disinfection technologies can be directly influenced by water quality. Generally, turbidity in treated water required more consumables for each of the technologies to ensure proper disinfection. These consumables can have a direct influence on overall sustainability. The requirements for capital along with operation and maintenance maybe help to inform the deployment of these POU technologies in various contexts. For example, chlorination relies heavily on the supply chain of NaOC1. Whereas the UV systems require readily available electricity. This level of our analysis revealed that water type can impact sustainability and requirements of each technology may present different opportunities for deployment.

4.2 Elucidating drivers of sustainability

The next level of analysis was to perform sensitivity analysis through Spearman's rank coefficient. This analysis was done for all POU technologies with water type 1 and water type 2 (Figure 14) to identify key parameters driving the sustainability. The key drivers are listed on the ordinate with the corresponding net cost and net GWP for all the POU technologies on the abscissa. The size of the circles is used to represent the magnitude of the Spearman's rank correlation coefficient. The absolute value of the correlation is reported between 1 and 0, with 1 having the most influence on the indicator. In this study, we are interested in the top key drivers with a Spearman's rank correlation of > 0.05. In cases where the correlation of many parameters is above 0.05, the top 5 parameters are reported.

4.3.1 Elucidating drivers for net cost. We report key net cost drivers for each technology for water type 1 and type 2, starting with the parameter with highest influence followed by subsequent key drivers. For water type 1 and 2, the key drivers for cost of POU chlorination were dose of NaOCl and price of NaOCl (Appendix Table A 9). This result is expected since NaOCl is the main consumable. The drivers for AgNP CWF with water type 1 were labor cost, discount rate, bucket cost, lid cost, and spout cost. With water type 2, labor cost, discount rate, bucket cost, AgNP, and lid cost. With AgNP CWF the labor cost had the greatest impact on cost for both water types. While most of key drivers for cost of the AgNP CWF were capital cost, water type 2 also had AgNP as a key driver because this water type required more frequent recoating of AgNP (Appendix Table A 10). Key drivers of cost with water type 1 for UV mercury lamp were unit cost and discount rate. For water type 2, the key drivers were unit cost, discount rate, lamp cost, and lamp lifespan. For water type 2, the lamps were required to be on for more time which led to more frequent replacement. The costs of UV LED system with water type 1 and 2 were impacted by unit cost and discount rate (Appendix Table A 11 and Table A 12). For both UV systems, a driver to their costs were unit costs. These UV systems are inherently a more expensive option compared to chlorination and AgNP CWF. However, it is notable that electricity cost did not significantly influence the sustainability of the UV systems.

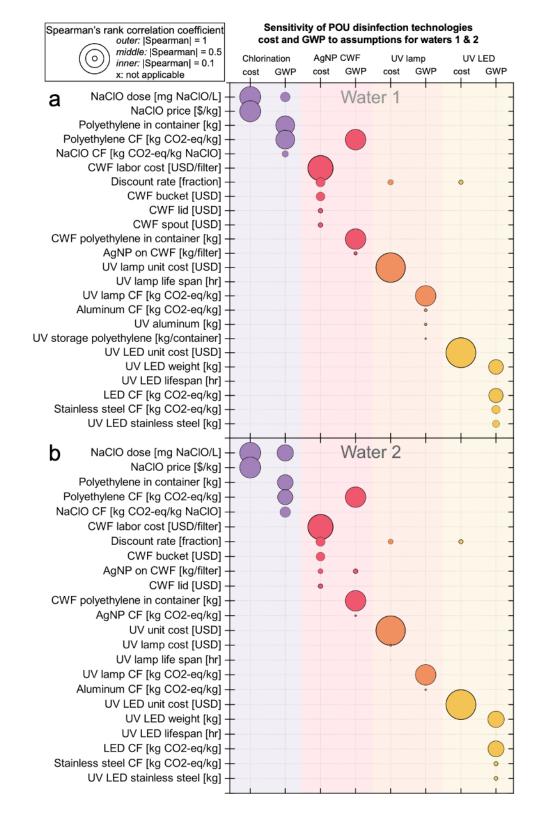


Figure 14. Spearman's rank correlation for net cost and GWP for all POU technologies with water type 1 (a) and water type 2 (b). The key drivers are on the ordinate corresponding with each technology's cost and GWP on the abscissa.

4.3.2 Elucidating drivers for GWP. The key drivers of GWP for each technology is reported for water type 1 and 2. The key GWP drivers for POU chlorination with water type 1 were polyethylene (PE) of container weight, PE impact factor, NaOCl dose, and NaOCl impact factor. With water type 2, NaOCl dose, PE of container weight, PE impact factor, and NaOCl impact factor. It is expected that the NaOCl dose influences the environmental impact because it is the main consumable of POU chlorination which impacts its maintenance and operation. The 20 L plastic container also had significant impact on LCA of POU chlorination system for both water type as a capital component of the system (Appendix Table A 9).

For water type 1, AgNP CWF key drivers were PE impact factor, PE in container, and AgNP loading. For water type 2, PE impact factor, PE in container, AgNP loading, and AgNP impact factor. AgNP loading is the concentration of AgNP on the CWF based on the mass of AgNP applied per filter (Appendix Table A 2).⁶⁶ The component with the highest influence on environmental impact of AgNP CWF system was the plastic bucket that holds the water that filters through the CWF. The AgNP coating had more influence on water type 2 due to the shorter AgNP lifespan which results in more frequent recoating of AgNP with the more turbid water (Appendix Table A 10).

UV mercury lamp key drivers for water type 1 were UV mercury lamp lifespan, UV mercury lamp impact factor, aluminum impact factor, aluminum foil weight, and PE from storage. For water type 2, the key drivers were UV mercury lamp lifespan, UV mercury lamp impact factor, and aluminum impact factor (Appendix Table A 11). The key drivers of the UV mercury lamp system were capital requirements and lamp replacement. The UV lamps are key drivers of GWP and can be attributed to the lamp's mercury content and the release of mercury into the environment during disposal considered a factor.⁷⁹ For the UV LED system with water type 1 and 2, the key drivers were LED weight, LED lifespan, LED impact factor, stainless steel impact factor, and stainless steel weight (Appendix Table A 12). Both UV systems had impact of lamp and LED lifespan because of the need for lamp replacement.

Overall, the results from the sensitivity analysis highlight how assumptions can impact financial and environmental sustainability. The identification of key drivers can also inform technology developers about key areas to research in order to improve sustainability. For example, when deploying POU chlorination using WaterGuard or similar products as a source of NaOC1, then the desired dose of NaOC1 will be the most important factor to consider while adjusting for cost and environmental impacts. The cost of the AgNP CWF was mostly impacted by labor; therefore, mass production of AgNP CWF may further reduce their cost. Generally, the additional required components beyond the ceramic and AgNPs were drivers for its sustainability, i.e., the GWP of the plastic containers along with the costs of bucket, lid and spout. The highest impact on cost for both UV systems was the unit cost; therefore, it will be beneficial for UV POU technologies to explore how they can be developed with a lower price. The negative Spearman's rank correlation of GWP impact of lamp and LED lifespan on GWP shows that an improvement in the lifespan can increase environmental sustainability. These key drivers can provide a potential pathway for technology developers and manufacturers to improve the sustainability of these POU technologies.

4.3 Short to long-term adoption of POU technologies

To explore the sustainability of the POU technologies for short to long-term adoption, the impact of length of adoption lifetime was explored. The adoption lifetime is the length of time (years) which the POU technology is expected to be used for by a household. In some cases, a POU technology may be needed for short-term deployment (e.g., disasters intervention). In other cases, it could be deployed throughout a community for long-term usage and treatment intervention especially in developing regions. For all the POU technologies the cost and environment impacts are reported for 1 to 15 years adoption and usage. The median along with the 5th, 25th, 75th, and 95th are reported. Across all POU technologies, we observed that the yearly per capita cost (Appendix Table A 13) and environmental impact (Appendix Table A 14) decreases as the lifetime increases. Broadly, this trend shows that the technologies are more sustainable with long-term adoption and usage. Long-term adoption is more beneficial because as the years go by, the cost and environmental impact of using the technologies is spread out rather than investing in the technology and only using it for few years. Although, the reduction in costs and environmental impacts with lifetimes varies significantly for the different POU technologies.

The net cost and GWP for POU chlorination in Figure 15 shows that all values were lower with long-term adoption. In short-term adoption of 1 year, the POU chlorination system had a net cost of 1.56 USD·cap⁻¹·yr⁻¹ and net GWP of 0.46 kg CO₂ eq·cap⁻¹·yr⁻¹ for the median estimates. Long-term adoption of 15 years has a decreased cost of 1.31 USD·cap⁻¹·yr⁻¹. The magnitude of decrease between the shortterm and long-term adoption net cost for the POU chlorination system is not very drastic. The similar cost over the increase in lifetime can be attributed to the continuous need for consumables to run the system (i.e., NaOCl). On the other hand, the GWP for 15 years adoption decreases to 0.07 kg CO₂ eq·cap⁻¹·yr⁻¹ from 0.46 kg CO₂ eq·cap⁻¹·yr⁻¹ for the 1-year adoption. This reduction in GWP with adoption is because the capital requirements of the 20 L jerry can are distributed over the lifetime. If cost is important for a particular context, these results reveal that POU chlorination may be a good solution for short-term adoption.

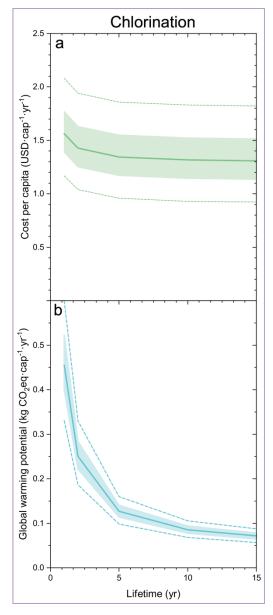


Figure 15: Impact of short to long-term adoption of POU chlorination on (a) cost and (b) global warming potential (GWP).. The cost and GWP are plotted over lifetime (years) of adoption. The median values are plotted as the center line, 25th and 75th percentiles are plotted in the shaded region, and 5th and 95th percentiles are plotted with the dashed lines.

The AgNP CWF system has lower net cost and GWP than all the other technologies over the entire spectrum of adoption length (Figure 16). Specifically, the estimated net cost for a 1-year adoption term was 2.20 USD cap⁻¹· yr⁻¹ and the net GWP was 0.22 kg CO₂ eq·cap⁻¹· yr⁻¹. Both the net cost and GWP reduced significantly as the years of adoption increased from 1 to 5. And at 15 years, the estimated net

cost and GWP were 0.20 USD·cap⁻¹·yr⁻¹ and 0.016 kg CO₂ eq·cap⁻¹·yr⁻¹, respectively. Therefore, for both short-term and long-term adoption, AgNP CWF system maybe with a viable option. This system has the potential to be the most sustainable option to adopt considering both cost and environmental impacts.

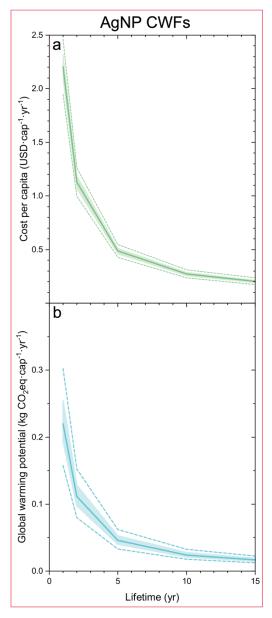


Figure 16: Impact of short to long-term adoption of silver nanoparticle enabled ceramic water filters (AgNP CWFs) on (a) cost and (b) global warming potential (GWP). The cost and GWP are plotted over lifetime (years) of adoption. The median values are plotted as the center line, 25th and 75th percentiles are plotted in the shaded region, and 5th and 95th percentiles are plotted with the dashed lines.

Both UV systems had a more drastic decline in cost and GWP with an increase in lifetime. This finding is due to the high capital requirements of these advanced systems. In other words, the longer the term of adoption for these systems allows for the capital requirements to be spread out over a longer period of time. Specifically, a 1-year adoption period of UV mercury lamp system had a net cost and GWP of 16.35 USD·cap⁻¹·yr⁻¹ and 3.42 kg CO₂ eq·cap⁻¹·yr⁻¹, respectively (Figure 17). These estimates reduced significantly after approximately 5 years, with 15 years adoption had a net cost of 1.56 USD·cap⁻¹·yr⁻¹ and GWP of 1.57 kg CO₂ eq·cap⁻¹·yr⁻¹.

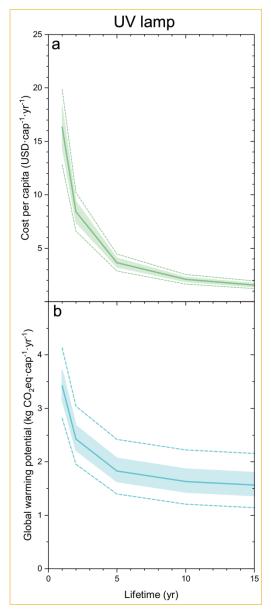


Figure 17: Impact of short to long-term adoption of UV lamp system on (a) cost and (b) global warming potential (GWP). The cost and GWP are plotted over lifetime (years) of adoption. The median values are plotted as the center line, 25th and 75th percentiles are plotted in the shaded region, and 5th and 95th percentiles are plotted with the dashed lines.

The UV LED system had the highest cost of all the technologies over the entire simulation space for adoption period (Figure 18). With 1 year adoption, the UV LED had a net cost of 43.21 USD \cdot cap⁻¹ \cdot yr⁻¹ ¹ while 15-year adoption had a net cost was 3.86 USD \cdot cap⁻¹ \cdot yr⁻¹. The GWP was 2.17 kg CO₂ eq \cdot cap⁻¹ \cdot yr⁻¹ for 1 year adoption and 0.50 kg CO₂ eq \cdot cap⁻¹ \cdot yr⁻¹ for 15 years. As with the other technologies the values decreased as the years of adoption increase as shown in. These results reveal that it is best to strive for long-term adoption when considering the UV systems.

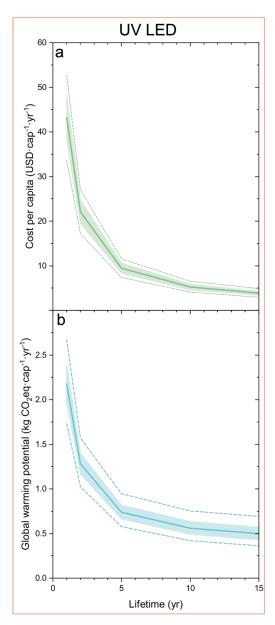


Figure 18: Impact of short to long-term adoption of UV LED system on (a) cost and (b) global warming potential (GWP). The cost and GWP are plotted over lifetime (years) of adoption. The median values are plotted as the center line, 25th and 75th percentiles are plotted in the shaded region, and 5th and 95th percentiles are plotted with the dashed lines.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Study limitations

This study evaluated sustainability based on cost and environmental impacts. However, other sustainability indicators may be considered in the future. Specifically, this study set disinfection efficacy to explore cost and environmental impacts. Given a certain cost or environmental matrices constrain, the disinfection efficacy of POU technologies can also be evaluated as an indicator for technology selection. Additionally, other microorganisms could be considered beyond *E. coli* for case specific situations, e.g., *cryptosporidium*. Different microbes will require different disinfection efficacy which will impact both the type of POU to select, the cost requirement and the environmental impact that will be accumulated. For example, chlorination may not be an effective method for some pathogens and other pathogens may require longer exposure time to disinfection. Another factor not considered is the potential for disinfection byproducts to form, which could be important for systems like POU chlorination. Therefore, understanding the potential byproducts associated with each system could be another measure that can shape decision making.

Some technological parameters and decision variables can also impact the outcome of the study. For example, the lamp lifespan for both UV systems can have an impact on the cost and environmental impacts, as better outcomes are expected for lamps with higher lifespan. Therefore, exploring the lifespans of UV lamps as specified by different manufacturers creates a better understanding of the sustainability of these systems. Moreover, the wattage of the UV lamps could also vary, which will influence energy requirements. For turbid waters with a high number of particles, pretreatment with particle removal might be important. Although the addition of pretreatment options like filtration would be an additional unit with more capital requirements, it may have other tradeoffs, e.g., can improve disinfection efficiency. Transportation of the water from the source to the household is another factor not

considered in this study. For example, if the raw water source is groundwater, considering the cost of well construction and groundwater pumping can influence the overall capital and energy requirements.

5.2 Conclusions

The QSD framework was leveraged for this study to reveal how POU technologies perform against each other in terms of cost and environmental impacts. From the economic analysis, the POU technology with the lowest net cost was AgNP CWF and the highest cost was UV LED system, under the baseline general set of assumptions. For environmental impacts, the AgNP CWF also had the lowest GWP while the UV (mercury lamp) system had the highest environmental impacts, under the baseline general set of assumptions. The water quality for water type 2 (which had higher turbidity) had a direct impact on the sustainability of these systems especially for operational and maintenance. If the motivation for selecting a technology is affordability (e.g., in low-income areas), POU chlorination would be appropriate for short-term adoption and AgNP CWF would be appropriate for long-term adoption. If GWP is the deciding factor for selecting a technology, AgNP CWF would be appropriate based on the reported low environmental impacts, according to the finding of this study. It is notable that the AgNP CWF is also easy to use; however, the process of recoating the AgNPs to the CWF will require an expert compared to POU chlorination that households can easily use without needing an expert.

Another major comparison in this study was the sustainability of UV mercury lamps versus UV LED. From this study, we estimate that UV LED had the higher cost under all adoption periods. However, UV LED had lower environmental impacts compared to UV mercury lamps. The relatively high GWP of UV mercury lamps are aligned with other studies and can be attributed to the disposal phase of the mercury of the lamps.⁷⁹ However, due to electricity demand both UV systems would be less effective in regions where electricity supply is not adequate or unavailable.

The disinfection of more turbid water also resulted in higher net GWP for all POU technologies. This finding is attributed to more replaceable components or consumables that are required in order to achieve adequate disinfection. Overall, these results give an understanding of the potential cost and environmental impacts while deploying a selected POU technology to households with similar water quality parameters modeled in this study. It also highlights the importance of technology developers to evaluate the impact of different water sources on the sustainability of their systems. It is notable that this study is not limited to only the water quality types used here as this framework can be applied to any reallife water quality. Evaluation of a specific water quality can be completed by updating the raw water data and script.

The sensitivity analysis resulted in an understanding of which of parameters in each POU technology are key drivers of the indicators of costs and GWP. Therefore, if these key drivers are controllable within a desired range, they can be used to potentially reduce cost and environmental impacts where necessary. The key drivers are also influenced by the water quality as some water quality parameters may affect the adjustment of these key drivers, e.g., adjusting NaOCl dose which is a key driver in POU chlorination to suit the turbidity of the raw water. The sensitivity analysis will in future allow for the selection of key drivers for each POU technology and then having a range of input values for the drivers to further access the drivers' individual impacts on the cost and environmental impacts of the technologies.

While this this study focused on four POU technologies that were selected, this framework can be adopted to explore other POU technologies including novel and emerging ones that need to be evaluated before deploying. This study has the potential to help inform research, development, and deployment of POU disinfection technologies. Specifically, decision makers, non-profit organizations, and future researchers may use these results and methods to help decide what POU technologies to deploy, while considering decision variables, technological variables, and contextual parameters. An important aspect of sustainability that can further inform decision making when selecting POU technologies is not only limited to economic (cost effectiveness) and performance of technology but the environmental of the POU technologies accumulated throughout its lifetime from manufacturing to usage to disposal is vital to decision making. Understanding environmental impacts of all stages of the POU technologies and identifying the key drivers (e.g., materials, components) for environmental impacts can help decision makers select and deploy eco-friendly systems.

It is important to note that the results and outcomes for both cost and environmental impacts of the POU technologies reported in this study are under a set of assumptions with uncertainty included on many of them. The assumptions are based on manufacturer's recommendations as well as published reports and papers. The specific results and outcomes can vary depending on the changes in key assumptions and parameters that drive sustainability. Also, the inclusion of additional decision variables, contextual parameters, and technological parameters may yield different outcomes, e.g., cost of transportation of water from source or pumping energy required for groundwater. The addition of other parameters or changes in parameters and assumptions can be incorporated into the future analysis to achieve better informed case-specific results. Therefore, this study can serve as a tool for which parameters and assumptions can be explored to better decision making in a specific context. The framework of this study is available as a blueprint to serve this purpose for future researchers and entities interested in understanding the relative sustainability of different POU technologies.

5.3 Recommendations

In this study, models and algorithms were developed so that all POU technologies have a disinfection efficacy of at least 3 log reduction. In the future of studies, the next criteria for relative sustainability for the POU technologies could be to set the model and algorithms to have typical use conditions and evaluate the disinfection efficacy across water types. The water types could also be modelled based on actual tested water samples in a context of interest to derive the water quality parameters that serve as raw water. Other contextual analysis could also be completed with location-specific data, e.g., price of materials and electricity.

In this study, the four POU technologies were modeled based on previous research and manufacturer's guidelines. In the future, this developed framework can be expanded to explore commercially available POU technologies as well as novel ones. Since the estimates of financial and environmental sustainability rely on assumptions, lab-scale studies on disinfection efficacy of POU technologies could be conducted in parallel to gain real-time results. Due to POU chlorination being a popular option in many underserved communities, future studies may evaluate other commercially available POU chlorination.

Adoption period was observed to have a drastic impact on the sustainability of the AgNP CWF and both UV systems. However, it is unclear if these technologies are guaranteed to survive the long-term adoption of 10 to 15 years. Therefore, a need exists to evaluate and improve technologies' lifetime and durability for long-term adoption.

The most sustainable POU technology option from the findings in this study is AgNP CWF because of the relatively low cost and environmental impacts. It is also relatively easy to use and can be useful in developing countries and places without adequate electricity. The POU chlorination will be best for short-term adoption like distribution of WaterGuard after a disaster. The unit costs of both UV systems are key drivers for the high cost. If the UV systems could be made available for lower unit cost, then it would be an effective POU for areas where the supply of electricity is guaranteed. Lower unit costs would make the UV LED more attractive for deployment because of its already relatively low environmental impacts. The results from this study can potentially inform decision makers, non-profit organizations, and future research on sustainable approaches to safe drinking water through POU technologies.

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APPENDIX

DATA FOR TECHNOLOGY AND RAW WATER SCRIPTS

Table A 1: Data set for the POU chlorination script. The dataset covers materials cost and design parameters. Uncertainty is added to the datapoint, and the data source is cited.

parameter	unit	expected	low	high	distribution	references
NaOCl _dose	mg NaOCl	1.87	1.4025	2.3375	uniform	74
	/L					
contact_time	min	30	22.5	37.5	uniform	74
container_cost	USD	1.6	1.2	2	uniform	91
container_volume	L	20			constant	74
container_vol	L/container	20			constant	74
NaOCl_cost	USD/kg	1.96	1.47	2.45	uniform	9F2
NaOCl_volume	L/bottle	0.15			constant	74
NaOCl _density	kg/L	1.21			constant	92
Rate_coefficient	•	3.2185			constant	93
Intercept		0.0845			constant	93
PE_in_container	kg	0.9	0.675	1.125	uniform	94
PE_to_ NaOCl	KgPE/kgN	0.096			constant	
	aOCl					
NaOCl _bottle_mass	kg	0.023	0.0172	0.0287	uniform	95

parameter	unit	expected	low	high	distribution	references
CWF_cost	USD	16.68	8	35	triangular	66
Clay_mass	kg	4.7	3.525	5.875	uniform	66
Sawdust_mass	kg	1.3	0.975	1.625	uniform	66
CWF_water	kg	2	1.5	2.5	uniform	66
AgNP	kg/filter	0.000064	9.6E- 06	0.000096	uniform	66
Electricity	Mj	0.0324	0.0243	0.0405	uniform	66
Brush_cost	USD	0.4	0.3	0.5	uniform	96
Wood_mass	kg	6.1	4	9.4	triangular	66
propane	kg	0.9	0.55	1.3	triangular	66
PE_in_container	kg	0.9	0.675	1.125	uniform	94
AgNP_low_lifetime	yr	1	0.5	1.5	uniform	97
AgNP_lifetime	yr	3	1.5	4.5	uniform	97
CWF_clay_cost	USD/filter	0.99	0.7425	1.2375	uniform	10
CWF_grog_cost	USD/filter	0.18	0.135	0.225	uniform	10
CWF_sawdust_cost	USD/filter	0.9	0.675	1.125	uniform	10
CWF_AgNP_cost_old	USD/filter	10	7.5	12.5	uniform	10
CWF_water_cost	USD/filter	0.02	0.015	0.025	uniform	10
CWF_wood_cost	USD/filter	0.5	0.375	0.625	uniform	10
CWF_labor_cost	USD/filter	5.53	4.1475	6.9125	uniform	10
CWF_additional_cost	USD/filter	4	3	5	uniform	10
CWF_AgNP_cost	USD/kg	1250	1000	1500	triangular	10
Argenol_AgNP_content	fraction Ag	0.725	0.7	0.75	triangular	98
CWF_bucket	USD	2	1.5	2.5	uniform	10
CWF_lid	USD	1	0.75	1.25	uniform	10
CWF_spout	USD	1	0.75	1.25	uniform	10

Table A 2: Dataset for the AgNP CWF script. The dataset covers materials cost and design parameters. Uncertainty is added to the datapoint, and the data source is cited.

parameter	unit	expected	low	high	distribution	references
uv_dose	mJ/cm2	187	140.25	233.75	uniform	78
UVT	%	95			constant	78
uv_unit_cost	USD	90	67.5	112.5	uniform	78
uv_flow	L/min	9.46	7.095	11.825	uniform	78
quartz_tube_volume	L	1.54			constant	78
uv_lamp_cost	USD	26	19.5	32.5	uniform	78
lamp_life_span	hr	2000	1500	2500	uniform	78
uv_PVC	kg	0.384405	0.288304	0.480507	uniform	78
uv_aluminum_foil	kg	0.391631	0.293723	0.489539	uniform	78
storage_PE	kg/container	0.9	0.675	1.125	uniform	94
uv_storage_cost	USD	1.6	1.2	2	uniform	91
uv_electric_cost	USD/l	0.000015	1.13E-05	1.88E-05	uniform	78
uv_electric_demand	W	30	22.5	37.5	uniform	78
number_of_uv_lamps	number of lamps	2			constant	78

Table A 3: Date for the UV mercury lamp system script. The dataset covers materials cost and design parameters. Uncertainty is added to the datapoint, and the data source is cited.

parameter	unit	expected	low	high	distribution	references
UVT	%	88			constant	79
uv_led_unit_cost	USD	245	183.75	306	uniform	79
uv_led_electric_cost	USD	0.2	0.15	0.25	uniform	79
uv_led_flow	L/min	0.19	0.1425	0.2375	uniform	80
uv_led_cost	USD	26	19.5	32.5	uniform	99
uv_led_lifespan	hr	10000	7500	12500	uniform	79
uv_led_per_unit		30			constant	80
uv_led_storage_cost	USD	1.6	1.2	2	uniform	91
uv_led_quartz	kg	0.081236	0.060927	0.101546	uniform	80
StainlessSteel	kg	1.328596	0.996447	1.660745	uniform	80
uv_led_dose	mJ/cm2	187	95	215	uniform	80
led_electricity_demand	W	23	11	35	uniform	81
uv_quartz	kg	0.233106	0.17483	0.291383	uniform	80
uv_led_weight	kg	0.0105	0.007875	0.013125	uniform	84
uv_led_storage_PE	kg/container	0.9	0.675	1.125	uniform	94

Table A 4: Data for the UV LED system script. The dataset covers materials cost and design parameters. Uncertainty is added to the datapoint, and the data source is cited.

RAW WATER DATA

Table A 5: Data for the raw water scripts for water types 1 and 2. The dataset covers water quality parameters. Uncertainty is added to the datapoint, and the data source is cited.

Water type 1									
parameter	unit	expected	low	high	distribution	references			
E_coli	CFU/mg	200000	150000	250000	uniform	10			
Turbidity	NTU	5	1	10	uniform	100			
ТОС	mg/L	5	1	10	uniform	101			
Ca	mg/L	30	20	40	uniform	78			
Mg	mg/L	30	20	40	uniform	78			
UVT	%	80	72	88	uniform	78			
Water type 2									
		W	ater type 2						
parameter	unit	Wa expected	ater type 2 low	high	distribution	references			
parameter E_coli	unit CFU/mg		• •		distribution uniform	references			
-		expected	low	high					
E_coli	CFU/mg	expected 200000	low 150000	high 250000	uniform	10			
E_coli Turbidity	CFU/mg NTU	expected 200000 20	low 150000 10	high 250000 30	uniform uniform	10 100			
E_coli Turbidity TOC	CFU/mg NTU mg/L	expected 200000 20 10	low 150000 10	high 250000 30 15	uniform uniform uniform	10 100 101			

ENVIRONMENTAL IMPACT DATA

Table A 6: Data for the global warming potential assumptions. The GWP impact dataset covers all
materials accounted for in all the POU technologies and their GWP. Uncertainty is added to each GWP
datapoint, and the data source is Ecoinvent version 3.

ID	unit	expected	low	high	distribution	references
Plastic	kg CO2-eq	1.97	1.93	2.01	uniform	ecoinvent 3
StainlessSteel	kg CO2-eq	4.33	3.07	5.5	uniform	ecoinvent 3
StainlessSteelSheet	kg CO2-eq	4.98	3.65	6.21	uniform	ecoinvent 3
Steel	kg CO2-eq	2.55	2.13	3.15	uniform	ecoinvent 3
Wood	kg CO2-eq	197	186	208	uniform	ecoinvent 3
PE	kg CO2-eq	2.7933	2.094975	3.491625	uniform	ecoinvent 3
PVC	kg CO2-eq	2.4204	1.8153	3.0255	uniform	ecoinvent 3
Uvlamp	kg CO2-eq	0.98118	0.735885	1.226475	uniform	ecoinvent 3
Aluminum	kg CO2-eq	15.106	11.3295	18.8825	uniform	ecoinvent 3
CWFClay	kg CO2-eq	0.010238	0.0076785	0.0127975	uniform	ecoinvent 3
SilverNP	kg CO2-eq	496.58	372.435	620.725	uniform	ecoinvent 3
Sawdust	kg CO2-eq	0.022008	0.016506	0.02751	uniform	ecoinvent 3
Quartz	kg CO2-eq	0.035012	0.026259	0.043765	uniform	ecoinvent 3
LED	kg CO2-eq	247.43	185.5725	309.175	uniform	ecoinvent 3

COST AND ENVIRONMENTAL IMPACTS RESULTS

Table A 7: Cost and environmental impacts of all POU technologies for water type 1. The capital cost and impact along with the operation and maintenance is reported. The net cost and GWP is reported for median, 5th and 95th percentiles.

Cost (USD/person/yr)						
	Capital	O&M	Net	Net	Net	
	0.5	0.5	0.5	0.05	0.95	
Chlorination	0.060738	1.283698	1.343758	0.957294	1.858157	
AgNP CWFs	0.478542	0.007487	0.486057	0.427573	0.546768	
UV lamp	3.538284	0.113657	3.651957	2.877123	4.435757	
UV LED	9.418379	0.025355	9.445701	7.350754	11.57297	
GWP (kg CO2 ed	q/person/yr)					
	Capital	O&M	Net	Net	Net	
	0.5	0.5	0.5	0.05	0.95	
Chlorination	0.082326	0.043595	0.126664	0.098408	0.159651	
AgNP CWFs	0.04575		0.04575	0.033197	0.062311	
UV lamp	1.82893	2.44E-05	1.828954	1.397715	2.419888	
UV LED	0.73728	0.001855	0.739011	0.578779	0.9449	

Cost (USD/person/yr)						
	Capital	O&M	Net	Net	Net	
	0.5	0.5	0.5	0.05	0.95	
Chlorination	0.060738	2.567396	2.627024	1.853205	3.653796	
AgNP CWFs	0.478542	0.009983	0.48868	0.429612	0.549477	
UV lamp	3.538284	0.227313	3.769893	2.988969	4.555864	
UV LED	9.418379	0.050709	9.472372	7.375421	11.59792	
GWP (kg CO2 ed	q/person/yr)					
	Capital	O&M	Net	Net	Net	
	0.5	0.5	0.5	0.05	0.95	
Chlorination	0.082326	0.087189	0.171144	0.135583	0.210311	
AgNP CWFs	0.046491		0.046491	0.033819	0.063158	
UV lamp	3.26527	4.87E-05	3.265314	2.412833	4.440827	
UV LED	1.113818	0.003709	1.116961	0.837988	1.507276	

Table A 8: For water type 2, Cost and environmental impacts of all POU technologies. The capital cost and impact along with the operation and maintenance is reported. The net cost and GWP is reported for median, 5th and 95th percentiles.

SPEARMAN'S RANK CORRELATION

Table A 9: The POU chlorination elucidating drivers of cost and environmental impacts for water type 1 and 2.

	Water type 1		
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission GlobalWarming [kg CO2-eq/cap/yr]
Cost drivers			
POUChlorination- D2	POUChlorination na cl O dose [mg NaOCl /L]	0.697672758	0.321712659
TEA	Na cl O price [\$/kg]	0.696512422	0.007003118
Environmental Imp	act drivers		
POUChlorination- D2	POUChlorination PE in container [kg]	0.000151108	0.638242064
LCA	PECF [kg CO2-eq/kg]	-0.003290513	0.632973612
POUChlorination- D2	POUChlorination na cl O dose [mg NaOCl /L]	0.697672758	0.321712659
LCA	Na cl O CF [kg CO2-eq/kg NaOCl]	0.007432278	0.208663532
	Water type 2		
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission GlobalWarming [kg CO2-eq/cap/yr]
Cost drivers	·	•	
POUChlorination- D2	POUChlorination na cl O dose [mg NaOCl /L]	0.698040069	0.546422424
TEA	Na cl O price [\$/kg]	0.69670675	0.005211194
Environmental Imp			
POUChlorination- D2	POUChlorination na cl O dose [mg NaOCl /L]	0.698040069	0.546422424
POUChlorination- D2	POUChlorination PE in container [kg]	0.00013754	0.520873919
LCA	PECF [kg CO2-eq/kg]	-0.003282974	0.510566032
LCA	Na cl O CF [kg CO2-eq/kg NaOCl]	0.00733244	0.342606148

Table A 10: The AgNP CWF elucidating drivers of cost and environmental impacts for water type 1 and 2.

Water type 1						
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission Global Warming [kg CO2-eq/cap/yr]			
Cost drivers						
Ag NP CWF-E2	[USD/filter]		0.010045256			
TEA	Discount rate [fraction]	0.297466173	0.008647642			
Ag NP CWF-E2	Ag NP CWF CWF bucket [USD]	0.288301484	-0.012002875			
Ag NP CWF-E2	Ag NP CWF CWF lid [USD]	0.150716757	0.005424618			
Ag NP CWF-E2	Ag NP CWF CWF spout [USD]	0.150511715	-0.012144317			
Environmental Im	nact drivers					
LCA	PECF [kg CO2-eq/kg]	0.005613189	0.692434037			
Ag NP CWF-E2	Ag NP CWF PE in container [kg]	0.005274619	0.690624295			
Ag NP CWF-E2	Ag NP CWF ag NP [kg/filter]	0.131052888	0.115754665			
	Water type	2				
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission Global Warming [kg CO2-eq/cap/yr]			
Cost drivers						
Ag NP CWF-E2	Ag NP CWF CWF labor cost [USD/filter]	0.841242361	0.009899368			
ТЕА	Discount rate [fraction]	0.296568487	0.009354402			
Ag NP CWF-E2	Ag NP CWF CWF bucket [USD]	0.28625171	-0.012485334			
Ag NP CWF-E2	Ag NP CWF ag NP [kg/filter]	0.161096169	0.153072101			
Ag NP CWF-E2	Ag NP CWF CWF lid [USD]	0.149791451	0.005405378			
Environmental Im	pact drivers					
LCA	PECF [kg CO2-eq/kg]	0.005627551	0.688492853			
Ag NP CWF-E2	Ag NP CWF PE in container [kg]	0.005023137	0.686115121			
Ag NP CWF-E2	Ag NP CWF ag NP [kg/filter]	0.161096169	0.153072101			
LCA	Silver NPCF [kg CO2-eq/kg]	-0.005950382	0.055777106			

Table A 11: The UV mercury lamp elucidating drivers of cost and environmental impacts for water type 1 and 2.

Water type 1						
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission GlobalWarming [kg CO2-eq/cap/yr]			
Cost drivers						
POU UV-F2	POU UV uv unit cost [USD]	0.984266068	0.003402151			
TEA	Discount rate [fraction]	0.172380557	-0.004251059			
Environmental Im	pact drivers					
POU UV-F2	POU UV lamp life span [hr]	-0.027884877	-0.692570502			
LCA	Uvlamp CF [kg CO2-eq/kg]	0.013095629	0.68549558			
LCA	Aluminum CF [kg CO2-eq/kg]	0.001546707	0.093446362			
POU UV-F2	POU UV uv aluminum foil [kg]	-0.016709272	0.080701604			
POU UV-F2	POU UV storage PE [kg/container]	0.018578889	0.057378977			
	Water type 2	2				
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission GlobalWarming [kg CO2-eq/cap/yr]			
Cost drivers	·					
POU UV-F2	POU UV uv unit cost [USD]	0.981071005	0.003788621			
TEA	Discount rate [fraction]	0.171528522	-0.003297773			
POU UV-F2	POU UV uv lamp cost [USD]	0.068916114	0.006925562			
POU UV-F2	POU UV lamp life span [hr]	-0.060013704	-0.699861973			
Environmental Im	pact drivers					
POU UV-F2	POU UV lamp life span [hr]	-0.060013704	-0.699861973			
LCA	Uvlamp CF [kg CO2-eq/kg]	0.013228547	0.694485695			
LCA	Aluminum CF [kg CO2-eq/kg]	0.001839643	0.049623777			

Table A 12: The UV LED system elucidating drivers of cost and environmental impacts for water type 1 and 2.

Water type 1						
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission GlobalWarming [kg CO2-eq/cap/yr]			
Cost drivers						
UV LED-G2	UV LED uv led unit cost [USD]	0.986385591	-0.00658818			
ТЕА	Discount rate [fraction]	0.144093629	0.006110942			
Environmental im	pact drivers					
UV LED uv led weight [kg]		0.00565815	0.49189166			
UV LED-G2	UV LED uv led lifespan [hr]	0.006995662	-0.487656131			
LCA	LEDCF [kg CO2-eq/kg]	0.003151922	0.482832808			
LCA	Stainless steel CF [kg CO2-eq/kg]	-0.010684992	0.269847466			
UV LED-G2	UV LED stainless steel [kg]	0.001132612	0.239248612			
	Water type 2	2				
Element	Parameter	Annual net cost [USD/cap/yr]	Net emission GlobalWarming [kg CO2-eq/cap/yr]			
Cost drivers						
UV LED-G2	UV LED uv led unit cost [USD]	0.986379275	-0.004820943			
TEA	Discount rate [fraction]	0.144046078	0.004267631			
Environmental im						
UV LED-G2	UV LED uv led weight [kg]	0.005668012	0.546357919			
UV LED-G2	UV LED uv led lifespan [hr]	0.004588971	-0.54177728			
LCA	LEDCF [kg CO2-eq/kg]	0.003124014	0.536282638			
LCA	Stainless steel CF [kg CO2-eq/kg]	-0.010719161	0.143617873			
UV LED-G2	UV LED stainless steel [kg]	0.001146859	0.128025071			

Table A 13: Short to long-term adoption of POU technologies impact on net cost. The median, 5th, 25th,
75th, and 95th percentiles are reported.

POU chlorination	Cost (USD/person/yr)				
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	1.167956	1.388022	1.561561	1.772851	2.082073
2	1.038692	1.25249	1.426285	1.634991	1.942223
5	0.957294	1.170626	1.343758	1.55265	1.858157
10	0.93021	1.14378	1.316783	1.526758	1.83073
15	0.921689	1.135221	1.308121	1.518093	1.821344
AgNP CWF		Cost	t (USD/perso	n/yr)	
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	1.947508	2.0808	2.203011	2.326258	2.460089
2	0.997073	1.066429	1.129416	1.192501	1.262561
5	0.427573	0.458845	0.486057	0.513403	0.546768
10	0.236753	0.256693	0.272871	0.28923	0.311387
15	0.173296	0.189769	0.202838	0.216246	0.235739
UV mercury lamp		Cost	t (USD/perso	n/yr)	
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	12.82011	14.38766	16.35056	18.31724	19.86041
2	6.606427	7.414023	8.412404	9.420827	10.20473
5	2.877123	3.232014	3.651957	4.085377	4.435757
10	1.631513	1.840713	2.081569	2.31473	2.544622
15	1.2165	1.3846	1.560699	1.735407	1.932872
UV LED		Cost	t (USD/perso	n/yr)	
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	33.63525	37.93089	43.20641	48.52585	52.79409
2	17.20528	19.40444	22.08831	24.8093	26.99849
5	7.350754	8.296213	9.445701	10.58933	11.57297
10	4.056335	4.611002	5.244675	5.880415	6.507177
15	2.96248	3.397293	3.867497	4.331567	4.870263

POU chlorination	GWP (kg CO2 eq/person/yr)				
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	0.330578	0.399723	0.455509	0.522494	0.614061
2	0.186032	0.221151	0.250095	0.283514	0.329669
5	0.098408	0.113994	0.126664	0.14037	0.159651
10	0.067791	0.077458	0.085572	0.09361	0.105155
15	0.05679	0.064869	0.071655	0.078356	0.087766
AgNP CWF	GWP (kg CO2 eq/person/yr)				
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	0.157783	0.193295	0.220028	0.254218	0.302395
2	0.079969	0.097689	0.111123	0.128198	0.152416
5	0.033197	0.040327	0.04575	0.052687	0.062311
10	0.01761	0.021158	0.023995	0.027507	0.032418
15	0.012299	0.014742	0.016756	0.019109	0.022461
UV mercury lamp	GWP (kg CO2 eq/person/yr)				
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	2.816548	3.15747	3.423061	3.709218	4.134955
2	1.953647	2.215276	2.426826	2.674541	3.040913
5	1.397715	1.63134	1.828954	2.064684	2.419888
10	1.206399	1.436591	1.632646	1.86229	2.220406
15	1.142566	1.368958	1.566765	1.796176	2.154193
UV LED	GWP (kg CO2 eq/person/yr)				
Lifetime (years)	0.05	0.25	0.5	0.75	0.95
1	1.731573	1.98275	2.174308	2.378709	2.675004
2	1.022558	1.168171	1.280341	1.395218	1.56914
5	0.578779	0.66801	0.739011	0.814605	0.9449
10	0.418115	0.493619	0.557698	0.629401	0.752532
15	0.362228	0.434611	0.497143	0.567332	0.690498

Table A 14: Short to long-term adoption of POU technologies impact on net GWP. The median, 5th, 25th, 75th, and 95th percentiles are reported.

POU CHLORINATION SCRIPT

#!/usr/bin/env python3
-*- coding: utf-8 -*"
QSDsan: Quantitative Sustainable Design for sanitation and resource recovery systems
Copyright (C) 2020, Quantitative Sustainable Design Group
This module is developed by:

Bright Elijah

beo5055@georgiasouthern.edu & brightcarlelijah@gmail.com>

Department of Civil Engineering and Construction

Georgia Southern University

This module is under the University of Illinois/NCSA Open Source License.

Please refer to https://github.com/QSD-Group/QSDsan/blob/master/LICENSE.txt

for license details.

""

%%

import numpy as np

from qsdsan import SanUnit, Construction

from qsdsan.utils.loading import load_data, data_path

from qsdsan.sanunits._decay import Decay

import os

from math import ceil, pi

from . import Decay

from .. import SanUnit, Construction

from ..utils import ospath, load_data, data_path

__all__ = ('POUChlorination',)
#path to csv with all the inputs
#data_path += '\sanunit_data/_pou_chlorination.tsv'
poucl_path = ospath.join(data_path, 'sanunit_data/_pou_chlorination.csv')
class POUChlorination(SanUnit):

"'mh

Point of use water treatment technology: Desinfection through chlorination

Reference documents

Hussein, M.; Brown, J.; Njee, R. M.; Clasen, T.; Malebo, H. M.; Mbuligwe, S. Point-of-Use Chlorination of Turbid Water: Results from a Field Study in Tanzania. Journal of Water and Health 2015, 13 (2), 544–552. http://dx.doi.org/10.2166/wh.2014.001

Tamene, A. A Qualitative Analysis of Factors Influencing Household Water Treatment Practices Among Consumers of Self-Supplied Water in Rural Ethiopia. Risk Management and Healthcare Policy 2021, 14, 1129–1139. https://doi.org/10.2147/RMHP.S299671.

Parameters

ins : Raw water

Chlorine

outs : Treated water

"

def __init__(self, ID=", ins=None, outs=(), thermo=None, init_with='WasteStream', number_of_households=1, **kwargs,):

SanUnit.__init__(self, ID, ins, outs, thermo, init_with)

self.number_of_households = number_of_households

load data from tsv each name will be self.name

```
data = load_data(path=poucl_path)
```

for para in data.index:

```
value = float(data.loc[para]['expected'])
```

setattr(self, para, value)

del data

for attr, value in kwargs.items():

```
setattr(self, attr, value)
```

define the number of influent and effluent streams

 $N_ins = 3$

 $N_outs = 1$

in _run: define influent and effluent streams and treatment processes

def _run(self):

raw_water, chlorine, Cl_bottle = self.ins

treated_water = self.outs[0]

give treated water all the properties and cmps of raw water

these will be changed below

treated_water.copy_like(self.ins[0])

chlorine.phase = 'l'

Cl_bottle.phase = 's'

add chlorine to the treated_water

#breakpoint()

if raw_water.turbidity <= 10:

pass

elif raw_water.turbidity > 10:

self. NaOCl _dose *= 2

chlorine.imass[' NaOCl '] = self. NaOCl _dose * treated_water.F_vol / 1000 # kg NaOCl /hr

self.chlorine_rate = chlorine.imass[' NaOCl ']

Cl_bottle.imass['Polyethylene'] = chlorine.imass[' NaOCl '] * self.PE_to_ NaOCl

disinfect bacteria from treated_water

Cl_Concentration = self. NaOCl_dose #mg/L

No = raw_water.imass['Ecoli']/raw_water.F_vol * 10**-4 # E coli CFU/ mL ICC/ml (intact cells counts) used by (Cheswick et al., 2020)

#_design will include all the construction or captial impacts

def _design(self):

design = self.design_results

defining the quantities of materials/items

note that these items are in the _impacts_items.xlsx data

design['PE'] = Container = self.number_of_households * self.PE_in_container

self.construction = (

Construction(item='PE', quantity = Container, quantity_unit = 'kg'),

)

self.add_construction(add_cost=False)

#_cost based on amount of steel and stainless plus individual components

def _cost(self):

#purchase_costs is used for capital costs

#can use quantities from above (e.g., self.design_results['StainlessSteel'])
#can be broken down as specific items within purchase_costs or grouped (e.g., 'Misc. parts')
self.baseline_purchase_costs['WaterContainer'] = (self.container_cost)*self.number_of_households
self.F_BM = dict.fromkeys(self.baseline_purchase_costs.keys(), 1)

#certain parts need to be replaced based on an expected lifefime
#the cost of these parts is considered along with the cost of the labor to replace them

AGNP CWF SCRIPT

#!/usr/bin/env python3
-*- coding: utf-8 -*""

QSDsan: Quantitative Sustainable Design for sanitation and resource recovery systems

Copyright (C) 2020, Quantitative Sustainable Design Group

This module is developed by:

Bright Elijah <be05055@georgiasouthern.edu>

Department of Civil Engineering and Construction

Georgia Southern University

This module is under the University of Illinois/NCSA Open Source License.

Please refer to https://github.com/QSD-Group/QSDsan/blob/master/LICENSE.txt

for license details.

•••

%%

import numpy as np
from qsdsan import SanUnit, Construction
from qsdsan.utils.loading import load_data, data_path
from qsdsan.sanunits._decay import Decay
import os

from math import ceil, pi #from . import Decay #from .. import SanUnit, Construction from ..utils import ospath, load_data, data_path

__all__ = ('AgNP_CWF',) #path to csv with all the inputs #data_path += '\sanunit_data/_pou_chlorination.tsv' agnp_path = ospath.join(data_path, 'sanunit_data/_AgNP_CWF_2.csv') class AgNP_CWF(SanUnit): "'mh

Point of use water treatment technology: Desinfection through Silver Nanoparticles

Reference documents

Iii, R.; Stetson, L. Socially Embedded and Sustained Point-of-Use Disinfection : Enhancing Silver Nanoparticle Enabled Ceramic Water Filters with a Navajo Pottery Technique. Thesis, 2020. https://doi.org/10.26153/tsw/13860.

Mikelonis, A. M.; Rowles, L. S.; Lawler, D. F. The Effects of Water Chemistry on the Detachment and Dissolution of Differently Stabilized Silver Nanoparticles from Ceramic Membranes. Environ. Sci.: Water Res. Technol. 2020, 6 (5), 1347–1356. https://doi.org/10.1039/C9EW01141B.

Parameters

ins : Raw water

AgNP

outs : Treated water

""

def __init__(self, ID=", ins=None, outs=(), thermo=None, init_with='WasteStream', number_of_households=1, **kwargs,):

SanUnit.__init__(self, ID, ins, outs, thermo, init_with)

self.number_of_households = number_of_households

data = load_data(path=agnp_path)

for para in data.index:

value = float(data.loc[para]['expected'])

setattr(self, para, value)

del data

for attr, value in kwargs.items():

setattr(self, attr, value)

 $N_ins = 1$

 $N_outs = 1$

in _run: define influent and effluent streams and treatment processes

def _run(self):

raw_water, = self.ins
treated_water = self.outs[0]

give treated water all the properties and cmps of raw water

these will be changed below

treated_water.copy_like(self.ins[0])

#set the equation for log reduction following the Chick Watson Kinetic Model for log removal. Log(N/No) = -K*co*t

#This was adopted from <https://pubs.acs.org/doi/full/10.1021/es4026084>

#Here the log reduction value was set in the san sunit data (this wil be improved to accomodate changes in the raw water quality)

No = raw_water.imass['Ecoli']/raw_water.F_vol * 10**-4 # E coli CFU/ mL ICC/ml (intact cells counts) used by (Cheswick et al., 2020)

log_reduction = self.log_reduction_cwf

log_N = log_reduction + np.log10(No) #CFU/mL

 $N = 10^{**}(log_N)$

#set conditional statement for simulation to capture the impact of raw water quality parameters

self.hardness = raw_water.imass['Ca'] + raw_water.imass['Mg']

if raw_water._turbidity <= 10 and self.hardness <= 60:

self.AgNP_lifetime = 2

elif raw_water._turbidity > 10 or self.hardness > 60:

self.AgNP_lifetime = 1.5

elif raw_water._turbidity > 10 and self.hardness > 60:

self.AgNP_lifetime = 0.5

#_design will include all the construction or captial impacts

def _design(self):

design = self.design_results

defining the quantities of materials/items

note that these items to be to be in the _impacts_items.xlsx

design['CWFClay'] = CWF_clay = self.number_of_households * self.Clay_mass

design['SilverNP'] = AgNP = self.number_of_households * self.AgNP
design['Sawdust'] = Sawdust = self.number_of_households *self.Sawdust_mass
design['PE'] = Container = self.number_of_households * self.PE_in_container/2

self.construction = (

Construction(item='CWFClay', quantity = CWF_clay, quantity_unit = 'kg'),

Construction(item='SilverNP', quantity = AgNP, quantity_unit = 'kg', lifetime = self.AgNP_lifetime, lifetime_unit='yr'),

Construction(item='Sawdust', quantity = Sawdust, quantity_unit = 'kg'),

Construction(item='PE', quantity = Container, quantity_unit = 'kg')

)

self.add_construction(add_cost=False)

#_cost based on amount of steel and stainless plus individual components

def _cost(self):

#purchase_costs is used for capital costs

#can use quantities from above (e.g., self.design_results['StainlessSteel'])

#can be broken down as specific items within purchase_costs or grouped (e.g., 'Misc. parts')

self.baseline_purchase_costs['brush'] = (self.Brush_cost)*self.number_of_households self.baseline_purchase_costs['clay'] = (self.CWF_clay_cost)*self.number_of_households self.baseline_purchase_costs['grog'] = (self.CWF_grog_cost)*self.number_of_households self.baseline_purchase_costs['sawdust'] = (self.CWF_sawdust_cost)*self.number_of_households self.baseline_purchase_costs['water'] = (self.CWF_water_cost)*self.number_of_households self.baseline_purchase_costs['wood'] = (self.CWF_water_cost)*self.number_of_households self.baseline_purchase_costs['wood'] = (self.CWF_wood_cost)*self.number_of_households self.baseline_purchase_costs['labor'] = (self.CWF_labor_cost)*self.number_of_households self.baseline_purchase_costs['labor'] = (self.CWF_labor_cost)*self.number_of_households self.baseline_purchase_costs['AgNP'] = (self.CWF_AgNP_cost*self.AgNP/self.Argenol_AgNP_content)*self.number_of_households

self.baseline_purchase_costs['Bucket'] = (self.CWF_bucket)*self.number_of_households self.baseline_purchase_costs['Lid'] = (self.CWF_lid)*self.number_of_households self.baseline_purchase_costs['Spout'] = (self.CWF_spout)*self.number_of_households self.F_BM = dict.fromkeys(self.baseline_purchase_costs.keys(), 1)

#certain parts need to be replaced based on an expected lifefime

#the cost of these parts is considered along with the cost of the labor to replace them

USD/yr

replacement_cost = (self.CWF_AgNP_cost*self.AgNP/self.Argenol_AgNP_content) * self.number_of_households / self.AgNP_lifetime

#self.add_OPEX = self.chlorine_rate / self. NaOCl _density / self.container_vol *
self.operator_refill_cost # USD/hr (all items are per hour)

 $self.add_OPEX = replacement_cost / (365*24)$

UV MERCURY LAMP SCRIPT

#!/usr/bin/env python3
-*- coding: utf-8 -*""

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be05055@georgiasouthern.edu & brightcarlelijah@gmail.com>

Department of Civil Engineering and Construction Georgia Southern University This module is under the University of Illinois/NCSA Open Source License. Please refer to https://github.com/QSD-Group/QSDsan/blob/master/LICENSE.txt for license details.

...

%%
import numpy as np
from qsdsan import SanUnit, Construction
from qsdsan.utils.loading import load_data, data_path
from qsdsan.sanunits._decay import Decay
import os
from math import ceil, pi
#from . import Decay
from .. import Decay
from .. import SanUnit, Construction
from ..utils import ospath, load_data, data_path
__all__ = ('POU_UV',)
#path to csv with all the inputs
#data_path += '\sanunit_data/_pou_chlorination.tsv'
pou_uv_path = ospath.join(data_path, 'sanunit_data/_pou_uv.csv')

class POU_UV(SanUnit):

"'mh

Point of use water treatment technology: Desinfection through POU UV

Reference documents

Younis, B. A.; Mahoney, L. E.; Yao, S. Field Evaluation of a Novel UV Water Disinfection System for Use in Underserved Rural Communities. *Water environment research : a research publication of the Water Environment Federation* 2018, 91 (1), 75–82. https://doi.org/10.2175/106143017x15131012188141. Parameters

ins : Raw water

outs : Treated water

.. N/A

...

def __init__(self, ID=", ins=None, outs=(), thermo=None, init_with='WasteStream', number_of_households=1, **kwargs,):

SanUnit.__init__(self, ID, ins, outs, thermo, init_with)

self.number_of_households = number_of_households

load data from tsv each name will be self.name

```
data = load_data(path=pou_uv_path)
```

for para in data.index:

value = float(data.loc[para]['expected'])

setattr(self, para, value)

del data

for attr, value in kwargs.items():

```
setattr(self, attr, value)
```

define the number of influent and effluent streams

There is one influent streams which is the raw water (from the raw water san unit)

The effluent stream is the treated water

 $N_ins = 1$

$$N_outs = 1$$

in _run: define influent and effluent streams and treatment processes

def _run(self):

raw_water, = self.ins

treated_water = self.outs[0]

give treated water all the properties and cmps of raw water

these will be changed below

treated_water.copy_like(self.ins[0])

if raw_water.F_vol > (self.uv_flow*60):

self.run_time = raw_water.F_vol/(self.uv_flow*60)

No = raw_water.imass['Ecoli']/raw_water.F_vol * 10**-4 # E coli CFU/ mL ICC/ml (intact cells counts) used by (Cheswick et al., 2020)

#set the equation for log reduction following the Chick Watson Kinetic Model for log removal. Log(N/No) = -K*co*t

#This was adopted from <https://escholarship.org/uc/item/3p76b9gb>

Chatterley, C.; Linden, K. Demonstration and Evaluation of Germicidal UV-LEDs for Point-of-Use Water Disinfection. Journal of Water and Health 2010, 8 (3), 479–486. https://doi.org/10.2166/wh.2010.124.

#Here the log reduction value was set in the san sunit data

log_removal = self.uv_slope*self.uv_dose + self.uv_intercept

log_N = log_removal + np.log10(No) #CFU/mL

 $N = 10^{**}(log_N)$

#set conditional statement for simulation to capture the impact of raw water quality parameters

if raw_water._turbidity <= 10:

self.lamp_lifespan_factor = 1

elif raw_water._turbidity > 10:

 $self.lamp_lifespan_factor = 0.5$

self.lamp_life_span *= self.lamp_lifespan_factor

#_design will include all the construction or captial impacts

def _design(self):

design = self.design_results

defining the quantities of materials/items

note that these items to be to be in the _impacts_items.xlsx

design['PE'] = uv_storage = self.number_of_households * self.storage_PE*2

design['PVC'] = uv_pvc = self.number_of_households * self.uv_PVC

```
design['Uvlamp'] = uv_lamp_mecury = self.number_of_households * self.number_of_uv_lamps
design['Aluminum'] = uv_aluminum_foil = self.number_of_households * self.uv_aluminum_foil
```

```
self.construction = (
```

Construction(item='PE', quantity = uv_storage, quantity_unit = 'kg'),

Construction(item='PVC', quantity = uv_pvc, quantity_unit = 'kg'),

Construction(item='Uvlamp', quantity = uv_lamp_mecury, quantity_unit = 'kg', lifetime = (self.lamp_life_span), lifetime_unit='hr'),

Construction(item='Aluminum', quantity = uv_aluminum_foil, quantity_unit = 'kg')

)

```
self.add_construction(add_cost=False)
```

#_cost based on amount of steel and stainless plus individual components

def _cost(self):

#purchase_costs is used for capital costs

#can use quantities from above (e.g., self.design_results['StainlessSteel'])

#can be broken down as specific items within purchase_costs or grouped

self.baseline_purchase_costs['uv_unit'] = (self.uv_unit_cost)*self.number_of_households self.baseline_purchase_costs['uv_storage'] = (self.uv_storage_cost*2)*self.number_of_households self.add_OPEX['uvlamp'] = (self.uv_lamp_cost/(self.lamp_life_span))

self.F_BM = dict.fromkeys(self.baseline_purchase_costs.keys(), 1)
power_demand = (self.uv_electric_demand / 1000) * self.run_time / self.lamp_lifespan_factor
self.power_utility(power_demand)

#certain parts need to be replaced based on an expected lifefime#the cost of these parts is considered along with the cost of the labor to replace them

UV LED SCRIPT

#!/usr/bin/env python3

-*- coding: utf-8 -*-

•••

QSDsan: Quantitative Sustainable Design for sanitation and resource recovery systems

Copyright (C) 2020, Quantitative Sustainable Design Group

This module is developed by:

Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com>

Department of Civil Engineering and Construction

Georgia Southern University

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Please refer to https://github.com/QSD-Group/QSDsan/blob/master/LICENSE.txt for license details.

...

%%
import numpy as np
from qsdsan import SanUnit, Construction
from qsdsan.utils.loading import load_data, data_path
from qsdsan.sanunits._decay import Decay
import os
from math import ceil, pi
#from . import Decay
from .. import SanUnit, Construction
from ..utils import ospath, load_data, data_path

__all__ = ('UV_LED',)

#path to csv with all the inputs
#data_path += '\sanunit_data/_pou_chlorination.tsv'
uv_led_path = ospath.join(data_path, 'sanunit_data/_uv_led.csv')

class UV_LED(SanUnit):

""mh

Point of use water treatment technology: Desinfection through UV LED

Reference documents

Chatterley, C.; Linden, K. Demonstration and Evaluation of Germicidal UV-LEDs for Point-of-Use Water Disinfection. Journal of Water and Health 2010, 8 (3), 479–486. https://doi.org/10.2166/wh.2010.124.

Jenny, R. M.; Simmons, O. D.; Shatalov, M.; Ducoste, J. J. Modeling a Continuous Flow Ultraviolet Light Emitting Diode Reactor Using Computational Fluid Dynamics. Chemical Engineering Science 2014, 116, 524.

Point-of-use water disinfection using ultraviolet and visible light-emitting diodes - PubMed. https://pubmed.ncbi.nlm.nih.gov/26967007/ (accessed 2023-02-13).

Parameters

ins : Raw water

outs : Treated water

•••

def __init__(self, ID=", ins=None, outs=(), thermo=None, init_with='WasteStream', number_of_households=1, **kwargs,):

SanUnit.__init__(self, ID, ins, outs, thermo, init_with)

self.number_of_households = number_of_households

load data from tsv each name will be self.name

data = load_data(path = uv_led_path)

for para in data.index:

value = float(data.loc[para]['expected'])

setattr(self, para, value)

del data

```
for attr, value in kwargs.items():
```

setattr(self, attr, value)

define the number of influent and effluent streams

There is one influent streams which is the raw water (from the raw water san unit)

The effluent stream is the treated water

 $N_ins = 1$

 $N_outs = 1$

in _run: define influent and effluent streams and treatment processes

def _run(self):

raw_water, = self.ins

treated_water = self.outs[0]

Give treated water all the properties and cmps of raw water

These will be changed below

treated_water.copy_like(self.ins[0])

No = raw_water.imass['Ecoli']/raw_water.F_vol * $10^{**}-4$ # E coli CFU/ mL ICC/ml (intact cells counts) used by (Cheswick et al., 2020)

#set the equation for log reduction following the Chick Watson Kinetic Model for log removal. Log(N/No) = -K*co*t

#This was adopted from <https://pubmed.ncbi.nlm.nih.gov/26179637/>

Chatterley, C.; Linden, K. Demonstration and Evaluation of Germicidal UV-LEDs for Point-of-Use Water Disinfection. Journal of Water and Health 2010, 8 (3), 479–486. https://doi.org/10.2166/wh.2010.124.

#Here the log reduction value was set in the san sunit data

log_removal = self.uv_led_slope*self.uv_led_dose + self.uv_led_intercept log_N = log_removal + np.log10(No) #CFU/mL N = 10**(log_N)

#set conditional statement for simulation to capture the impact of raw water quality parameters

if raw_water._turbidity <= 10: self.led_lifespan_factor = 1 elif raw_water._turbidity > 10: self.led_lifespan_factor = 0.5

self.uv_led_lifespan *= self.led_lifespan_factor

if raw_water.F_vol > (self.uv_led_flow*60):

self.run_time = raw_water.F_vol/(self.uv_led_flow*60)

#_design will include all the construction or captial impacts

def _design(self):

design = self.design_results

defining the quantities of materials/items

note that these items to be to be in the _impacts_items.xlsx

design['Quartz'] = uv_led_quartz = self.number_of_households * self.uv_quartz

design['PE'] = uv_led_storage = self.number_of_households * self.uv_led_storage_PE*2

design['StainlessSteel'] = uv_led_steel = self.number_of_households * self.StainlessSteel

design['LED'] = uv_led = self.number_of_households * self.uv_led_weight

self.construction = (

Construction(item='Quartz', quantity = uv_led_quartz, quantity_unit = 'kg'),

Construction(item='PE', quantity = uv_led_storage, quantity_unit = 'kg'),

Construction(item='StainlessSteel', quantity = uv_led_steel, quantity_unit = 'kg'),

```
Construction(item='LED', quantity = uv_led, quantity_unit = 'kg', lifetime = (self.uv_led_lifespan), lifetime_unit='hr'),
```

```
)
self.add_construction(add_cost=False)
```

def _cost(self):

#purchase_costs is used for capital costs

#can use quantities from above (e.g., self.design_results['StainlessSteel'])
#can be broken down as specific items within purchase_costs or grouped

self.baseline_purchase_costs['uv_led_unit'] = (self.uv_led_unit_cost)*self.number_of_households
self.baseline_purchase_costs['uv_led_storage'] =
(self.uv_led_storage_cost*2)*self.number_of_households

#self.baseline_purchase_costs['uv_pump'] = (self.uv_led_pump_cost)*self.number_of_households
self.add_OPEX['LED'] = (self.uv_led_cost/(self.uv_led_lifespan))

self.F_BM = dict.fromkeys(self.baseline_purchase_costs.keys(), 1)

power_demand = (self.led_electricity_demand / 1000) * self.run_time /self.led_lifespan_factor self.power_utility(power_demand)

#certain parts need to be replaced based on an expected lifetime#The cost of these parts is considered along with the cost of the labor to replace them

RAW WATER SCRIPT

#!/usr/bin/env python3

-*- coding: utf-8 -*-

•••

QSDsan: Quantitative Sustainable Design for sanitation and resource recovery systems This module is developed by:

Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com>

Department of Civil Engineering and Construction

Georgia Southern University

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for license details.

•••

%%

from .. import SanUnit

from ..utils import ospath, load_data, data_path

 $_all_ = ('RawWater',)$

raw_water_path = ospath.join(data_path, 'sanunit_data/_raw_water1.tsv')

#raw_water_path = ospath.join(data_path, 'sanunit_data/_raw_water2.tsv')

%%

class RawWater(SanUnit):

•••

References

Iii, R.; Stetson, L. Socially Embedded and Sustained Point-of-Use Disinfection : Enhancing Silver Nanoparticle Enabled Ceramic Water Filters with a Navajo Pottery Technique. Thesis, 2020. https://doi.org/10.26153/tsw/13860.

Stumm, W.; Morgan, J. J. Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters; Wiley, 1996.

Maciel, P. M. F.; Fava, N. de M. N.; Lamon, A. W.; Fernandez-Ibañez, P.; Byrne, J. A.; Sabogal-Paz, L. P. Household Water Purification System Comprising Cartridge Filtration, UVC Disinfection and Chlorination to Treat Turbid Raw Water. Journal of Water Process Engineering 2021, 43, 102203. https://doi.org/10.1016/j.jwpe.2021.102203.

Wilhelm, N.; Kaufmann, A.; Blanton, E.; Lantagne, D. Sodium Hypochlorite Dosage for Household and Emergency Water Treatment: Updated Recommendations. Journal of Water and Health 2017, 16 (1), 112–125. https://doi.org/10.2166/wh.2017.012.

Parameters _____ ins :none outs : Raw water ... $N_{ins} = 0$ N outs = 1def init (self, ID=", ins=None, outs=(), thermo=None, init with='WasteStream', household_size=6, number_of_households=1, water_demand=3.7, **kwargs): SanUnit.__init__(self, ID, ins, outs, thermo, init_with) self.household_size = household_size self.number of households = number of households self.water_demand = water_demand data = load_data(path=raw_water_path) for para in data.index: value = float(data.loc[para]['expected'])

```
setattr(self, para, value)
```

del data

for attr, value in kwargs.items():
 setattr(self, attr, value)

def _run(self):

water = self.outs[0]

water.empty()

factor = self.household_size * self.water_demand / 24 # from L per day of water to kg per hour

water.imass['Ecoli'] = self.E_coli/1000*factor

###! units are MPN/hr need to confirm this is done correctly

water._TOC = self.TOC # mg/L
water.imass['Ca'] = self.Ca/1000*factor # kg/hr
water.imass['Mg'] = self.Ca/1000*factor # kg/hr
water._turbidity = self.Turbidity # NTU
water.F_vol = factor
water._UVT = self.UVT # %

SYSTEMS SCRIPT FOR FOUR POU TECHNOLOGIES WITH TEA AND LCA

#!/usr/bin/env python3
-*- coding: utf-8 -*-

...

This module is developed by:

This module is developed by:

Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com>

Department of Civil Engineering and Construction

Georgia Southern University

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Please refer to https://github.com/QSD-Group/EXPOsan/blob/main/LICENSE.txt

for license details.

•••

%%

Filter out warnings related to solid content import warnings warnings.filterwarnings('ignore', message='Solid content') import graphviz as graphviz import numpy as np import biosteam as bst import piosteam as bst import qsdsan as qs from collections.abc import Iterable from sklearn.linear_model import LinearRegression as LR from qsdsan import sanunits as su from qsdsan import WasteStream, ImpactIndicator, ImpactItem, StreamImpactItem, SimpleTEA, LCA from exposan.POU_dis import results_path

from exposan.bwaise._cmps import cmps #from exposan.POU_dis._cmps import cmps from exposan.POU_dis._lca_data import lca_data_kind, load_lca_data, _ImpactItem_LOADED

```
#
==
# Unit parameters
#
==
currency = qs.currency = 'USD'
qs.CEPCI = qs.CEPCI_by_year[2018]
discount_rate = 0.05
qs.set_thermo(cmps)
household_size = 6
household\_per\_container = 1
get_pou_user = lambda: household_size * household_per_container
ppl_1k = 1000
ppl_{500} = 500
get_ppl = lambda kind: ppl_1k if kind=='1k' else ppl_500
lifetime_all= 5
#
==
# Prices and GWP CFs
#
==
==
price_dct = {
  'Electricity': 0.17,
  'Concrete': 194,
  'Steel': 2.665,
  ' NaOCl ': 1.96/0.15/1.21/0.125, #updated later
  'Polyethylene': 0, #update later
  }
GWP_dct = \{
```

```
'Electricity': 0.1135,
'CH4': 28,
'N2O': 265,
'N': -5.4,
NaOCl ': 2.6287,
'Polyethylene': 2.7933,
}
```

```
GWP = ImpactIndicator('GWP', unit='kg CO2')
bst.PowerUtility.price = price_dct['Electricity']
```

#ImpactItem.get_item(' NaOCl ').price = price_dct[' NaOCl ']

```
'OD2HH': 0.00134} # stratospheric ozone depletion to human health
```

```
H_factor = {'GW2ECO': 0.000000028, 'GW2HH': 0.000000928, 'OD2HH': 0.000531}
```

```
I_factor = {'GW2ECO': 0.000000025, 'GW2HH': 0.0000125, 'OD2HH': 0.000237}
```

StreamImpactItem(ID='CH4_item',

```
E_EcosystemQuality_Total=E_factor['GW2ECO']*4.8,
         E_HumanHealth_Total=E_factor['GW2HH']*4.8,
         H_EcosystemQuality_Total=H_factor['GW2ECO']*34,
         H_HumanHealth_Total=H_factor['GW2HH']*34,
         I_EcosystemQuality_Total=I_factor['GW2ECO']*84,
         I_HumanHealth_Total=I_factor['GW2HH']*84
         )
StreamImpactItem(ID='N2O_item',
         E_EcosystemQuality_Total=E_factor['GW2ECO']*78.8,
         # From climate change + ozone depletion
         E_HumanHealth_Total = 
           E_factor['GW2HH']*78.8+E_factor['OD2HH']*0.017,
         H_EcosystemQuality_Total=H_factor['GW2ECO']*298,
         H_HumanHealth_Total=\
           H_factor['GW2HH']*298+H_factor['OD2HH']*0.011,
         I EcosystemQuality Total=I factor['GW2ECO']*264,
         I_HumanHealth_Total=\
           I_factor['GW2HH']*264+I_factor['OD2HH']*0.007
         )
```

else:

```
raise ValueError(f`kind` can only be "original" or "new", not "{kind}".')
global _ImpactItem_LOADED
_ImpactItem_LOADED = True
```

```
NaOCl_item = StreamImpactItem(ID=' NaOCl_item', GWP=GWP_dct[' NaOCl '])
```

```
Polyethylene_item = StreamImpactItem(ID='Polyethylene_item', GWP=GWP_dct['Polyethylene'])
```

```
def batch_create_streams(prefix):
```

```
stream_dct = { }
```

item = ImpactItem.get_item('CH4_item').copy(f'{prefix}_CH4_item', set_as_source=True)

stream_dct['CH4'] = WasteStream(f'{prefix}_CH4', phase='g', stream_impact_item=item)

CH4.stream_impact_item = ImpactItem.get_item('CH4_item').copy(stream=CH4, set_as_source=True)

item = ImpactItem.get_item('N2O_item').copy(f'{prefix}_N2O_item', set_as_source=True)

stream_dct['N2O'] = WasteStream(f'{prefix}_N2O', phase='g', stream_impact_item=item)

N2O.stream_impact_item = ImpactItem.get_item('N2O_item').copy(stream=N2O, set_as_source=True)

 $item = ImpactItem.get_item('Polyethylene_item').copy(f'{prefix}_Polyethylene_item', set_as_source=True)$

stream_dct['Polyethylene'] = WasteStream(f'{prefix}_Polyethylene', phase='s',
price=price_dct['Polyethylene'],

stream_impact_item=item)

return stream_dct

%%

#

==

POU Chlorination (sysD): test system

#

==

flowsheetD = bst.Flowsheet('sysD')

bst.main_flowsheet.set_flowsheet(flowsheetD)

streamsD = batch_create_streams('D')

D1 = su.RawWater('D1', outs=('raw_water'), household_size=household_size, number_of_households=(get_ppl('1k')/household_size))

D2 = su.POUChlorination('D2', ins=(D1-0, streamsD[NaOCl '], streamsD['Polyethylene']), outs='treated_water', number_of_households=(get_ppl('1k')/household_size))

sysD.simulate()

#
==
AgNP CWF (sysE): test system
#

flowsheetE = bst.Flowsheet('sysE')
bst.main_flowsheet.set_flowsheet(flowsheetE)

streamsE = batch_create_streams('E')

E1 = su.RawWater('E1', outs=('raw_water'), household_size=household_size,

number_of_households=(get_ppl('1k')/household_size))

E2 = su.AgNP_CWF('E2', ins=(E1-0), outs='treated_water', number_of_households=(get_ppl('1k')/household_size))

sysE.simulate()

#
==
POU UV (sysF): test system
#
==

flowsheetF = bst.Flowsheet('sysF')
bst.main_flowsheet.set_flowsheet(flowsheetF)
streamsF = batch_create_streams('F')

F1 = su.RawWater('F1', outs=('raw_water'), household_size=household_size, number_of_households=(get_ppl('1k')/household_size)) F2 = su.POU_UV('F2', ins=(F1-0), outs='treated_water',

number_of_households=(get_ppl('1k')/household_size))

sysF = bst.System('sysF', path=(F1, F2))

sysF.simulate()

lcaF = LCA(system=sysF, lifetime=lifetime_all, lifetime_unit='yr', uptime_ratio=1, annualize_construction=True, E_item=lambda: F2.power_utility.rate*(365*12*5))

```
#
====
# UV LED (sysG): test system
#
===
```

flowsheetG = bst.Flowsheet('sysG')
bst.main_flowsheet.set_flowsheet(flowsheetG)
streamsG = batch_create_streams('G')

G1 = su.RawWater('G1', outs=('raw_water'), household_size=household_size,

 $number_of_households=(get_ppl('1k')/household_size))$

G2 = su.UV_LED('G2', ins=(G1-0), outs='treated_water',

number_of_households=(get_ppl('1k')/household_size))

sysG.simulate()

```
# %%
```

```
def update_lca_data(kind):
```

•••

Load impact indicator and impact item data.

Parameters

kind : str

"original" loads the data from Trimmer et al.

(TRACI, ecoinvent v3.2), "new" loads the data for ReCiPe and TRACI (ecoinvent 3.7.1, at the point of substitution).

```
global lca_data_kind
```

if lca_data_kind != kind: load_lca_data(kind) batch_create_stream_items(kind)

for lca in (lcaD, lcaE, lcaF, lcaG):
 for i in lca.lca_streams:
 # To refresh the impact items
 source_ID = i.stream_impact_item.source.ID
 i.stream_impact_item.source = ImpactItem.get_item(source_ID)

for i in sysD, sysE, sysF, sysG:
 i.simulate()

lca_data_kind = kind

def get_total_inputs(unit, multiplier=1):

```
if len(unit.ins) == 0: #
```

ins = unit.outs

else:

ins = unit.ins

inputs = $\{\}$

inputs[' NaOCl '] = sum(i.imass[' NaOCl '] for i in ins)

inputs['Polyethylene'] = sum(i.imass['Polyethylene'] for i in ins)

```
inputs['Ecoli'] = sum(i.Ecoli*i.F_vol/1e3 for i in ins)
```

```
for i, j in inputs.items():
    inputs[i] = j * multiplier
    return inputs
```

```
#breakpoint()
```

 $sys_dct = {$

```
'ppl': dict(sysD=get_ppl('1k'), sysE=get_ppl('1k'), sysF=get_ppl('1k'),sysG=get_ppl('1k')),
'input_unit': dict(sysD=D1, sysE=E1, sysF=F1, sysG=G1),
'liq_unit': dict(sysD=D1, sysE=E2, sysF=None, sysG=None),
'sol_unit': dict(sysD=None, sysE=E2, sysF=None, sysG=None),
'gas_unit': dict(sysD=None, sysE=None, sysF=None, sysG=None),
'stream_dct': dict(sysD=streamsD, sysE=streamsE, sysF=streamsF, sysG=streamsG),
'TEA': dict(sysD=teaD, sysE=teaE, sysF=teaF, sysG=teaG),
'LCA': dict(sysD=lcaD, sysE=lcaE, sysF=lcaF, sysG=lcaG),
'cache': dict(sysD={}, sysE={}, sysF={}, sysG={}),
}
```

def get_summarizing_functions(system):

 $func_dct = \{\}$

func_dct['get_annual_net_cost'] = lambda tea, ppl: (tea.EAC)/ppl

func_dct['get_annual_CAPEX'] = lambda tea, ppl: tea.annualized_CAPEX/ppl

func_dct['get_annual_OPEX'] = lambda tea, ppl: tea.AOC/ppl

```
ind = 'GlobalWarming'
```

 $func_dct['get_annual_GWP'] = \setminus$

lambda lca, ppl: lca.total_impacts[ind]/lca.lifetime/ppl

```
func\_dct['get\_constr\_GWP'] = \setminus
```

lambda sys, lca, ppl: (lca.get_stream_impacts(stream_items=lca.stream_inventory, kind='direct_emission')[ind]) \

/lca.lifetime/ppl

func_dct['get_other_GWP'] = \setminus

lambda lca, ppl: lca.total_other_impacts[ind]/lca.lifetime/ppl

#func_dct[' NaOCl '] = lambda sys: carbon_dict[' NaOCl '][sys.ID]

return func_dct

def print_summaries(systems):

try: iter(systems)

```
except: systems = (systems, )
```

for sys in systems:

func = get_summarizing_functions(sys)
sys.simulate()
ppl = sys_dct['ppl'][sys.ID]
print(f'\n------ Summary for {sys} ------\n')
tea = sys_dct['TEA'][sys.ID]
tea.show()

```
unit = f'{currency}/cap/yr'
print(f'\nNet cost: {func["get_annual_net_cost"](tea, ppl):.1f} {unit}.')
print(f'Capital: {func["get_annual_CAPEX"](tea, ppl):.1f} {unit}.')
print(f'Operating: {func["get_annual_OPEX"](tea, ppl):.1f} {unit}.')
print('\n')
```

```
lca = sys_dct['LCA'][sys.ID]
lca.show()
print('\n')
```

```
unit = f'{GWP.unit}/cap/yr'
```

print(f'\nNet emission: {func["get_annual_GWP"](lca, ppl):.2f} {unit}.')

print(f'Construction: {func["get_constr_GWP"](lca, ppl):.2f} {unit}.')

print(f'Transportation: {func["get_trans_GWP"](lca, ppl):.2f} {unit}.')

print(f'Stream items emission: {func["get_stream_items_emission_GWP"](sys, lca, ppl):.2f} {unit}.')

print(f'Other: {func["get_other_GWP"](lca, ppl):.2} {unit}.\n')

def save_all_reports():

import os

if not os.path.isdir(results_path):

os.path.mkdir(results_path)

```
for i in (sysD, sysE, lcaD, lcaE):
```

if isinstance(i, bst.System):

i.simulate()

i.save_report(os.path.join(results_path, f'{i.ID}_report.xlsx'))

else:

i.save_report(os.path.join(results_path, f'{i.system.ID}_lca.xlsx'))

```
\_all\_ = ('sysD', 'sysE', 'teaD', 'teaE', 'lcaD', 'lcaE', 'lcaD', 'lc
```

```
'print_summaries', 'save_all_reports',
*(i.ID for i in sysD.units),
*(i.ID for i in sysE.units)
)
```

MODELS SCRIPT

```
#!/usr/bin/env python3
```

```
# -*- coding: utf-8 -*-
```

```
•••
```

EXPOsan: Exposition of sanitation and resource recovery systems

This module is developed by:

Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com> Department of Civil Engineering and Construction Georgia Southern University This module is under the University of Illinois/NCSA Open Source License. Please refer to https://github.com/QSD-Group/EXPOsan/blob/main/LICENSE.txt for license details. "" # %% import os, pickle import numpy as np import pandas as pd from chaospy import distributions as shape from thermosteam.functional import V_to_rho, rho_to_V from biosteam import PowerUtility

from biosteam.evaluation import Model, Metric

from qsdsan import currency, ImpactItem

from qsdsan.utils import (

ospath, load_data, data_path, dct_from_str,

AttrSetter, AttrFuncSetter, DictAttrSetter,

FuncGetter,

time_printer

)

from exposan import POU_dis as pou

 $c_path = pou._lca_data.c_path$

```
lca_data_kind = pou.systems.lca_data_kind
__all__ = ('modelD','modelE','modelF','modelG')
##%%
##
==
# # Functions for batch-making metrics and -setting parameters
##
==
systems = pou.systems
sys_dct = systems.sys_dct
price_dct = systems.price_dct
GWP_dct = systems.GWP_dct
get_summarizing_functions = systems.get_summarizing_functions
def add LCA metrics(system, metrics, kind):
  systems.update_lca_data(kind)
  lca = sys_dct['LCA'][system.ID]
  ppl = sys_dct['ppl'][system.ID]
  funcs = [
    lambda ID: lca.total_impacts[ID]/lca.lifetime/ppl,
    lambda ID: lca.total_construction_impacts[ID]/lca.lifetime/ppl,
    lambda ID: lca.total_transportation_impacts[ID]/lca.lifetime/ppl,
    lambda ID: lca.get_stream_impacts(stream_items=lca.stream_inventory, kind='direct_emission')[ID]
\
       /lca.lifetime/ppl,
    lambda ID: lca.get_stream_impacts(stream_items=lca.stream_inventory, kind='offset')[ID] \
       /lca.lifetime/ppl,
    lambda ID: lca.total_other_impacts[ID]/lca.lifetime/ppl
    1
```

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for ind in lca.indicators:

```
unit = f'{ind.unit}/cap/yr'
cat = 'LCA results'
metrics.extend([
    Metric(f'Net emission {ind.ID}', FuncGetter(funcs[0], (ind.ID,)), unit, cat),
    Metric(f'Construction {ind.ID}', FuncGetter(funcs[1], (ind.ID,)), unit, cat),
    Metric(f'Transportation {ind.ID}', FuncGetter(funcs[2], (ind.ID,)), unit, cat),
    Metric(f'Direct emission {ind.ID}', FuncGetter(funcs[3], (ind.ID,)), unit, cat),
    Metric(f'Offset {ind.ID}', FuncGetter(funcs[4], (ind.ID,)), unit, cat),
    Metric(f'Other {ind.ID}', FuncGetter(funcs[5], (ind.ID,)), unit, cat),
    [])
```

return metrics

def add_metrics(system, kind):

sys_ID = system.ID
tea = sys_dct['TEA'][sys_ID]
ppl = sys_dct['ppl'][sys_ID]
func = get_summarizing_functions(system)

metrics = []

```
unit = f' \{ currency \} / cap/yr' \}
```

cat = 'TEA results'

metrics.extend([

Metric('Annual net cost', lambda: func['get_annual_net_cost'](tea, ppl), unit, cat), Metric('Annual CAPEX', lambda: func['get_annual_CAPEX'](tea, ppl), unit, cat), Metric('Annual OPEX', lambda: func['get_annual_OPEX'](tea, ppl), unit, cat),])

metrics = add_LCA_metrics(system, metrics, kind)

return metrics

#!!! leave out update_metrics for now, may need to add in later

def update_metrics(model, kind):

- # metrics = [i for i in model.metrics if i.element_name!='LCA results']
- # model.metrics = add_LCA_metrics(model.system, metrics, kind)
- # return model

def batch_setting_unit_params(df, model, unit, exclude=()):

for para in df.index:

if para in exclude: continue

b = getattr(unit, para)

```
lower = float(df.loc[para]['low'])
```

```
upper = float(df.loc[para]['high'])
```

```
dist = df.loc[para]['distribution']
```

```
if dist == 'uniform':
```

```
D = shape.Uniform(lower=lower, upper=upper)
```

```
elif dist == 'triangular':
```

```
D = shape.Triangle(lower=lower, midpoint=b, upper=upper)
```

```
elif dist == 'constant': continue
```

else:

```
raise ValueError(f'Distribution {dist} not recognized for unit {unit}.')
```

```
su_type = type(unit).__name__
```

```
if su_type.lower() == 'lagoon':
```

su_type = f'{unit.design_type.capitalize()} lagoon'

```
name = f'{su_type} {para}'
```

model.parameter(setter=AttrSetter(unit, para),

name=name, element=unit,

```
kind='coupled', units=df.loc[para]['unit'],
baseline=b, distribution=D)
```

```
#%%
```

#	
==	
# Shared by all systems	
#	
=======================================	
<pre>su_data_path = ospath.join(data_path, 'sanunit_data/')</pre>	
def add_shared_parameters(model, water):	
########### Related to multiple units ####################################	
sys = model.system	
######################################	
param = model.parameter	
streams = sys_dct['stream_dct'][sys.ID]	
tea = sys_dct['TEA'][sys.ID]	

Household size

- $b = systems.household_size$
- D = shape.Trunc(shape.Normal(mu=b, sigma=1.8), lower=1)
- @param(name='Household size', element=water, kind='coupled', units='cap/household',

baseline=b, distribution=D)

def set_household_size(i):

 $systems.household_size = i$

General TEA settings

Money discount rate

b = systems.discount_rate

D = shape.Uniform(lower=0.03, upper=0.06)

@param(name='Discount rate', element='TEA', kind='isolated', units='fraction',

baseline=b, distribution=D)

def set_discount_rate(i):

 $systems.discount_rate = tea.discount_rate = i$

Electricity price

```
b = price_dct['Electricity']
```

D = shape.Triangle(lower=0.08, midpoint=b, upper=0.21)

@param(name='Electricity price', element='TEA', kind='isolated',

units='\$/kWh', baseline=b, distribution=D)

def set_electricity_price(i):

```
PowerUtility.price = i
```

NaOCl price

```
b = price_dct[' NaOCl ']
```

D = shape.Uniform(lower=1.96/0.15/1.21/0.125*0.75, upper=1.96/0.15/1.21/0.125*1.25)

@param(name=' NaOCl price', element='TEA', kind='isolated',

units='\$/kg', baseline=b, distribution=D)

```
def set_ NaOCl_price(i):
```

```
price_dct['NaOCl'] = streams['NaOCl'].price = i
```

return model

def add_LCA_CF_parameters(model, kind=pou._lca_data.lca_data_kind):

param = model.parameter

sys = model.system

lca = sys_dct['LCA'][sys.ID]

LCA CF

if kind == 'original':

 $b = GWP_dct['CH4']$

D = shape.Uniform(lower=28, upper=34)

```
@param(name='CH4 CF', element='LCA', kind='isolated', units='kg CO2-eq/kg CH4',
```

baseline=b, distribution=D)

def set_CH4_CF(i):

GWP_dct['CH4'] = ImpactItem.get_item('CH4_item').CFs['GlobalWarming'] = i

 $b = GWP_dct['N2O']$

D = shape.Uniform(lower=265, upper=298)

@param(name='N2O CF', element='LCA', kind='isolated', units='kg CO2-eq/kg N2O',

baseline=b, distribution=D)

def set_N2O_CF(i):

 $GWP_dct['N2O'] = ImpactItem.get_item('N2O_item').CFs['GlobalWarming'] = i$

b = GWP_dct['Electricity']

```
D = shape.Uniform(lower=0.106, upper=0.121)
```

@param(name='Electricity CF', element='LCA', kind='isolated',

```
units='kg CO2-eq/kWh', baseline=b, distribution=D)
```

def set_electricity_CF(i):

GWP_dct['Electricity'] = ImpactItem.get_item('E_item').CFs['GlobalWarming'] = i

 $b = GWP_dct['NaOCl']$

D = shape.Triangle(lower=2.6287*0.75, midpoint=b, upper=2.6287*1.25)

@param(name='NaOCl CF', element='LCA', kind='isolated',

units='kg CO2-eq/kg NaOCl', baseline=b, distribution=D)

def set_NaOCl_CF(i):

GWP_dct['NaOCl'] = ImpactItem.get_item('NaOCl_item').CFs['GlobalWarming'] = i

b = GWP_dct['Polyethylene']

D = shape.Triangle(lower=2.7933*0.75, midpoint=b, upper=2.7933*1.25)

@param(name='Polyethylene CF', element='LCA', kind='isolated',

units='kg CO2-eq/kg Polyethylene', baseline=b, distribution=D)

def set_Polyethylene_CF(i):

GWP_dct['Polyethylene'] = ImpactItem.get_item('Polyethylene_item').CFs['GlobalWarming'] = i

 $\# b = GWP_dct['PVC']$

D = shape.Triangle(lower=1.0*0.75, midpoint=b, upper=1.0*1.25)

@param(name='PVC CF', element='LCA', kind='isolated',

units='kg CO2-eq/kg PVC', baseline=b, distribution=D)

def set_PVC_CF(i):

GWP_dct['PVC'] = ImpactItem.get_item('PVC_item').CFs['GlobalWarming'] = i

```
# b = GWP_dct['Mecury']
```

D = shape.Triangle(lower=1.0*0.75, midpoint=b, upper=1.0*1.25)

@param(name='Mecury CF', element='LCA', kind='isolated',

units='kg CO2-eq/kg Mecury', baseline=b, distribution=D)

def set_Mecury_CF(i):

GWP_dct['Mecury'] = ImpactItem.get_item('Mecury_item').CFs['GlobalWarming'] = i

b = GWP_dct['Aluminum']

D = shape.Triangle(lower=1.0*0.75, midpoint=b, upper=1.0*1.25)

@param(name='Aluminum CF', element='LCA', kind='isolated',

units='kg CO2-eq/kg Mecury', baseline=b, distribution=D)

def set_Aluminum_CF(i):

GWP_dct['Aluminum'] = ImpactItem.get_item('Aluminum_item').CFs['GlobalWarming'] = i

item_path = ospath.join(pou._lca_data.data_path, 'items_original.xlsx')

```
data = load_data(item_path, sheet='GWP')
```

for p in data.index:

```
item = ImpactItem.get_item(p)
```

b = item.CFs['GlobalWarming']

lower = float(data.loc[p]['low'])

upper = float(data.loc[p]['high'])

dist = data.loc[p]['distribution']

if dist == 'uniform':

```
D = shape.Uniform(lower=lower, upper=upper)
```

elif dist == 'triangular':

D = shape.Triangle(lower=lower, midpoint=b, upper=upper)

```
elif dist == 'constant': continue
```

else:

raise ValueError(f'Distribution {dist} not recognized.')

model.parameter(name=p+'CF',

setter=DictAttrSetter(item, 'CFs', 'GlobalWarming'),

element='LCA', kind='isolated',

units=f'kg CO2-eq/{item.functional_unit}',

baseline=b, distribution=D)

return model

#%%

#

==

```
# Scenario D (sysD)
```

==

==

sysD = systems.sysD
sysD.simulate()
modelD = Model(sysD, add_metrics(sysD, lca_data_kind))
paramD = modelD.parameter

Shared parameters

modelD = add_shared_parameters(modelD, systems.D1)

 $modelD = add_LCA_CF_parameters(modelD)$

RawWater

D1 = systems.D1 path = ospath.join(su_data_path, '_raw_water1.tsv') data = load_data(path) batch_setting_unit_params(data, modelD, D1)

Chlorination
D2 = systems.D2
path = ospath.join(su_data_path, '_pou_chlorination.csv')
data = load_data(path)
batch_setting_unit_params(data, modelD, D2)

##%%

##

==

Scenario E (sysE)

##

==

```
sysE = systems.sysE
sysE.simulate()
```

modelE = Model(sysE, add_metrics(sysE, lca_data_kind))

paramE = modelE.parameter

Shared parameters

 $modelE = add_shared_parameters(modelE, systems.E1)$

```
modelE = add_LCA_CF_parameters(modelE)
```

RawWater

E1 = systems.E1 path = ospath.join(su_data_path, '_raw_water1.tsv') data = load_data(path) batch_setting_unit_params(data, modelE, E1)

AgNP CWF

```
E2 = systems.E2

path = ospath.join(su_data_path, '_AgNP_CWF_2.csv')

data = load_data(path)

batch_setting_unit_params(data, modelE, E2)

# # %%
```

#

==

Scenario F (sysF)

#

==

sysF = systems.sysF sysF.simulate() modelF = Model(sysF, add_metrics(sysF, lca_data_kind)) paramF = modelF.parameter

Shared parameters
modelF = add_shared_parameters(modelF, systems.F1)
modelF = add_LCA_CF_parameters(modelF)

RawWater
F1 = systems.F1
path = ospath.join(su_data_path, '_raw_water1.tsv')
data = load_data(path)
batch_setting_unit_params(data, modelF, F1)

UV lamp
F2 = systems.F2
path = ospath.join(su_data_path, '_pou_uv.csv')
data = load_data(path)
batch_setting_unit_params(data, modelF, F2)

##%%

#
==
Scenario G (sysG)
#

```
sysG = systems.sysG
sysG.simulate()
modelG = Model(sysG, add_metrics(sysG, lca_data_kind))
paramG = modelG.parameter
```

Shared parameters
modelG = add_shared_parameters(modelG, systems.G1)
modelG = add_LCA_CF_parameters(modelG)

RawWater
G1 = systems.G1
path = ospath.join(su_data_path, '_raw_water1.tsv')
data = load_data(path)
batch_setting_unit_params(data, modelG, G1)

UV LED

G2 = systems.G2 path = ospath.join(su_data_path, '_uv_led.csv') data = load_data(path) batch_setting_unit_params(data, modelG, G2) # # %%

##

result_dct = {

'sysD': dict.fromkeys(('parameters', 'data', 'percentiles', 'spearman')),

```
'sysE': dict.fromkeys(('parameters', 'data', 'percentiles', 'spearman')),
'sysF': dict.fromkeys(('parameters', 'data', 'percentiles', 'spearman')),
'sysG': dict.fromkeys(('parameters', 'data', 'percentiles', 'spearman')),
}
```

@time_printer

```
def run_uncertainty(model, seed=None, N=1000, rule='L',
percentiles=(0, 0.05, 0.25, 0.5, 0.75, 0.95, 1),
spearman_metrics='default'):
```

if seed:

np.random.seed(seed)

```
samples = model.sample(N, rule)
```

```
model.load_samples(samples)
model.evaluate()
```

Spearman's rank correlation,

metrics default to net cost, net emission, and total recoveries

```
spearman_results = None
```

if spearman_metrics:

if spearman_metrics.lower() == 'default':

spearman_metrics = [i for i in model.metrics

if 'net' in i.name.lower() or 'total' in i.name.lower()]

Different versions of BioSTEAM

try: spearman_results = model.spearman_r(model.parameters, spearman_metrics)[0]
except: spearman_results = model.spearman_r(model.parameters, spearman_metrics)

spearman_results.columns = pd.Index([i.name_with_units for i in spearman_metrics])

dct = organize_uncertainty_results(model, spearman_results, percentiles) return dct

Data organization

def organize_uncertainty_results(model, spearman_results,

percentiles=(0, 0.05, 0.25, 0.5, 0.75, 0.95, 1)):

global result_dct

dct = result_dct[model._system.ID]

index_p = len(model.parameters)

dct['parameters'] = model.table.iloc[:, :index_p].copy()

```
dct['data'] = model.table.iloc[:, index_p:].copy()
```

if percentiles is not None:

dct['percentiles'] = dct['data'].quantile(q=percentiles)

if spearman_results is not None:

dct['spearman'] = spearman_results

return dct

def save_uncertainty_results(model, dct=None, path="):

if not path:

path = ospath.join(c_path, 'results')

if not ospath.isdir(path):

os.mkdir(path)

path = ospath.join(path, f'sys{model._system.ID[-1]}_model.xlsx')

elif not (path.endswith('xlsx') or path.endswith('xls')):

extension = path.split('.')[-1]

raise ValueError(f'Only "xlsx" and "xls" are supported, not {extension}.')

dct = dct or result_dct[model._system.ID]

if dct['parameters'] is None:

raise ValueError('No cached result, run model first.')

with pd.ExcelWriter(path) as writer:

dct['parameters'].to_excel(writer, sheet_name='Parameters')

dct['data'].to_excel(writer, sheet_name='Uncertainty results')

if 'percentiles' in dct.keys():

dct['percentiles'].to_excel(writer, sheet_name='Percentiles')
dct['spearman'].to_excel(writer, sheet_name='Spearman')
model.table.to_excel(writer, sheet_name='Raw data')

RESULTS AND SENSITIVITY ANALYSIS FOR ALL POU TECHNOLOGIES

-*- coding: utf-8 -*-

Created on Wed Mar 30 17:17:30 2022 Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com> Department of Civil Engineering and Construction Georgia Southern University """ ############POU chlorination from qsdsan import stats as a from exposan import stats as a from exposan import POU_dis as pou m = pou.models modelD = m.modelD uncertainty = m.run_uncertainty(modelD, seed=5, N=10000) m.save_uncertainty_results(modelD)

################ -*- coding: utf-8 -*-

Created on Wed Mar 30 17:17:30 2022 Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com> Department of Civil Engineering and Construction Georgia Southern University """ #AgNP CWF from qsdsan import stats as a from exposan import POU_dis as pou m = pou.models modelE = m.modelE uncertainty = m.run_uncertainty(modelE, seed=5, N=10000) m.save_uncertainty_results(modelE) # -*- coding: utf-8 -*-..... Created on Wed Aug 31 13:14:39 2022 Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com> Department of Civil Engineering and Construction Georgia Southern University ############ UV mercury lamp from qsdsan import stats as a from exposan import POU_dis as pou m = pou.modelsmodelF = m.modelFuncertainty = m.run_uncertainty(modelF, seed=5, N=10000) m.save_uncertainty_results(modelF) # -*- coding: utf-8 -*-..... Created on Wed Aug 31 13:14:40 2022 Bright Elijah <be05055@georgiasouthern.edu & brightcarlelijah@gmail.com> Department of Civil Engineering and Construction Georgia Southern University ########### UV LED

from qsdsan import stats as a from exposan import POU_dis as pou m = pou.models modelG = m.modelG uncertainty = m.run_uncertainty(modelG, seed=5, N=10000) m.save_uncertainty_results(modelG)