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The Sustainability of Ion Exchange Water Treatment Technology

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The Sustainability of Ion Exchange Water Treatment Technology

by

Adib Amini

A dissertation submitted in partial fulfillment
of the requirements for the degree of
Doctor of Philosophy in Environmental Engineering
Department of Civil and Environmental Engineering
College of Engineering
University of South Florida

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Abstract

This research investigated using a life cycle environmental and economic approach to evaluate IX technology for small potable water systems, allowing for the identification and development of process and design improvements that reduce environmental impacts and costs. The main goals were to evaluate conventional IX in terms of life cycle environmental and economic sustainability, develop a method for improving designs of IX systems from a environmental and economic sustainability standpoint, evaluate potential design improvements, and make the research findings accessible to water professionals through user-friendly tools and frameworks that take into account their feedback. This research provides an understanding, from the perspective of life cycle environmental impacts and costs, of the tradeoffs between various reactor designs of IX, the effects of scale, key contributors to impact and cost, design trends that improve sustainability, and how combined cation anion exchange compares to conventional IX. Furthermore, tools were developed that can be used to identify design choices that improve sustainability of IX systems. These tools were made into a user-friendly format to better bridge the gap between research and practice.

Chapter 1: Introduction

Human population growth and economic development are increasing water demands globally while increasing the scarcity of water sources (Vorosmarty et al., 2000). These increases in water demand as well as improved understanding of environmental impacts associated with water treatment highlight the need for sustainable water treatment technologies (European Environment Agency, 2012; UNEP and IWMI, 2012). Furthermore, potable water systems face numerous environmental and economic challenges in most regions of the world and in 2013 approximately one fourth of all potable water systems (PWS) in the U.S. were in significant violation of EPA or state rules (USEPA, 2013). This places increased responsibility on PWS to provide environmentally and economically sustainable water treatment.

Small PWS comprise the vast majority of all PWS and often face greater challenges and incur a higher number of legal violations (USEPA, 2013). This is because small PWS often have significantly less resources to operate and maintain their systems. For example, small PWS often have a small customer base, lack funds for implementation or maintenance of treatment systems, have staff that lack a high degree of expertise, and are geographically isolated. Therefore, a significant amount of assistance and resources are provided by the USEPA to small PWS to finance, operate, and maintain their systems (USEPA, 2013). Technologies are therefore needed that can meet the operational needs of small PWS while reducing environmental and economic impacts.

Ion exchange (IX) is a technology that can be used to remove hardness and a wide variety of contaminants from drinking water. IX provides effective and robust technical performance that is effective under varying water chemistry. IX is also a scalable technology that can be employed in centralized or decentralized systems, such as household treatment or a municipal drinking water facility. IX is also flexible in terms of operation mode, reactor configurations, and sequence in a treatment train. Therefore, IX's advantages provide opportunities for safe, effective, and affordable water treatment.

IX systems, however, can introduce environmental impacts and economic costs due to energy, chemicals, and other materials used throughout their life cycle. Energy usage is required for pumping and mixing, resin is required throughout the operation of the system, large amounts of salt may be necessary for regeneration of the resin, and brine waste resulting from the regeneration process requires disposal. These introduce a number of environmental burdens and incur significant costs in implementation of IX systems. Furthermore, waste brine can also impact external systems, such as wastewater treatment plants, where high salinity can affect plant operation (Maul et al., 2014; Panswad and Anan, 1999). Therefore, if not designed and managed properly, IX can provide significant disadvantages for small PWS.

As IX is becoming more prominent in small PWS (Ali and Gupta, 2007), it is essential to better understand the environmental and economic impacts of their construction and operation as well as developing methods for improving IX designs. Micro-economic and technical considerations have traditionally been paramount in the design of water treatment systems and the traditional approach involves use of design guides, practical experience, and short term cost analysis. However, improved methods are needed to better consider life cycle environmental and economic considerations in IX design.

Life cycle assessment (LCA) is a method of quantifying environmental impacts of systems and is a valuable tool for assessing the environmental sustainability of water treatment technology. Additionally, life cycle cost analysis (LCCA) provides a method for comprehensive economic evaluation of products, systems, and processes. Use of a life cycle approach helps to avoid shifting of environmental and economic burdens from one stage of the life cycle to another and helps to identify technological innovation opportunities. LCA, therefore, avoids the issues of only taking into account site-specific considerations (e.g. only emissions at a particular plant instead of due to the materials and processes upstream) (Azapagic et al., 1999).

Few studies have applied LCA to IX technology for drinking water treatment. These studies, as well as their main findings, are shown in Table 1.1. These studies have compared IX technology to other types of drinking water technology, such as RO, catalytic reduction, and adsorption, with target contaminants such as perchlorate, arsenic, nitrate, and hardness. However, the results from the previous studies are often context sensitive. None of the studies consider more than one system and installation, but varying management practices, operation, and environmental or design factors can significantly affect the environmental impacts of the system. Therefore, evaluation of a wider number of systems is needed to provide more complete understanding of how the impacts of the technology can differ in various circumstances. Furthermore, the impact of scale, the effect of common design and reactor configurations, and the influence of other IX design parameters have not been evaluated in previous studies.

Older studies have also evaluated the costs of IX technology (Clifford et al., 1987; Dahab, 1987; Richard, 1989; Rogalla et al., 1990; Andrews and Harward, 1994; Kapoor and Viraraghavan, 1997). However, design, operation, and costs have changed significantly over the past two decades and new IX innovations have not been evaluated. Furthermore, a life cycle approach is rarely used and LCCA of IX drinking water treatment has only been performed in one study (Choe et al., 2013).

Table 1.1: Studies that have applied LCA to IX drinking water technology

Author/Date	Systems Studied	Contaminant Removed	Main Findings
Ras and von Blottnitz (2012)	IX vs. RO	Hardness	• IX better in abiotic resource depletion and greenhouse gas emissions because of low electricity requirements • IX worse in human toxicity and freshwater aquatic ecotoxicity.
Choe et al. (2013)	IX vs. Biological Reduction w/ Acetate, Catalytic Reduction	Perchlorate	• Regeneration is most significant env. impact contributor of IX. • IX preferable to 2 alternatives (High impacts from electron donor production (acetate) and catalysts such as palladium and rhenium)
Dominguez et al. (2014)	IX vs. Adsorption	Arsenic	• IX has 13 times less primary resource and 17 times less environmental burdens
Choe et al. (2015)	Catalytic reduction to reuse IX brine	Nitrate	• Reuse of brine decreased impacts

In addition to evaluating the current state of the sustainability of IX, new methods are needed to for sustainable design improvement. Utilization of environmental sustainability for design improvement has been increasing (Azapagic, 1999; Azapagic et al., 2006) and the importance of systematically integrating LCA into process design rather than considering it as an ‘add on’ has been outlined (Azapagic et al., 2006). However, few tools exist for this purpose and LCA has never been directly tied to conventional design improvement methods, such as process modeling. Furthermore, LCCA has rarely been used in such approaches (Fazeni et al., 2015). Such tools could not only assist in identifying design trends that decrease environmental impacts and costs, but can also be used to evaluate novel IX technology designs.

Combined removal of multiple contaminants in IX is an example of a novel treatment design that shows great potential for reducing environmental and economic impacts. Conventionally, IX has been used for removal of a single contaminant and when multiple systems have been required to treat both cation and anionic contaminants. Combined IX has the potential to perform both types of treatment in a single process, while reducing material and energy requirements as well as waste during operation; however, no LCA or LCCA studies have been performed on these systems.

There is furthermore a recognized gap between science and practice (Bero et al., 1998; Bansal et al., 2012; Langrall, 2014) with research results often not reaching the intended community of practice. Researchers must therefore begin to research efforts the means to bridge the gap between that which is applicable (what is relevant) and that which is actionable (how to implement it in the world) (Argyris and Schon, 1974). Development of user-friendly tools as well as assessment frameworks that take into account user feedback are needed to allow research to better reach the community of practice.

The central hypothesis guiding this research is that using a life cycle environmental and economic approach can allow for the identification and development of process and design improvements to IX technology for small PWS that reduce environmental impacts and costs. Although this research focuses primarily on relatively small PWS, the findings of this research are relevant to most larger systems as well. The central hypothesis gives rise to four main goals that will be pursued in this research. These goals are also summarized in Figure 1.1.

- Goal 1: Evaluate conventional IX used in small potable water systems in terms of life cycle environmental and economic sustainability

- Goal 2: Develop a method of design improvement for IX systems that integrates environmental and economic sustainability
- Goal 3: Evaluate potential design improvements, such as combined IX removal, and compare to conventional IX technology
- Goal 4: Make the research findings accessible to water professionals through user-friendly tools that can be used in the field as well as assessment frameworks that take into account feedback from water professionals.

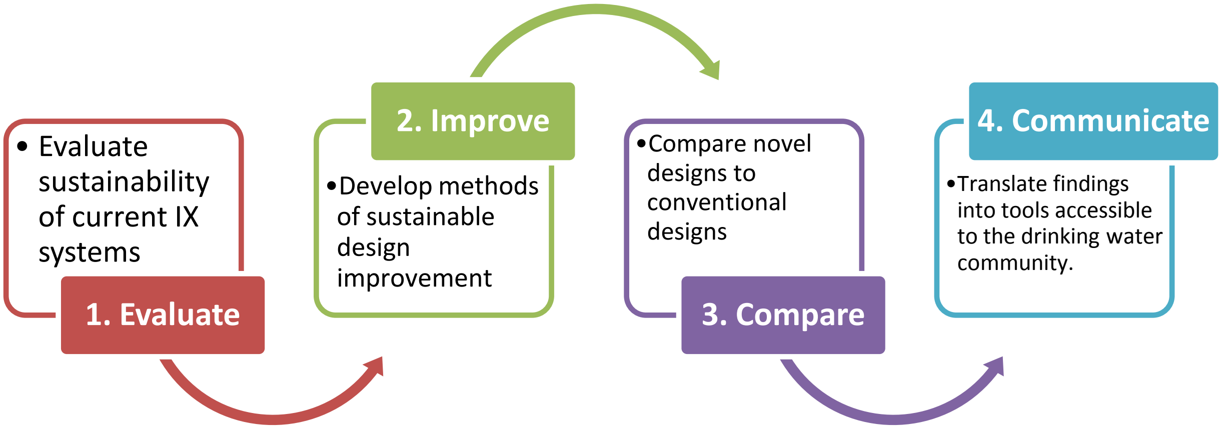

Figure 1.1: Diagram of four main goals of this research

Achievement of the four main goals translates into four primary tasks that will be accomplished in this research:

- Task 1: Perform LCA and cost analysis of IX plants in Florida
- Task 2: Develop and apply a model of IX systems that tightly integrates process modeling with LCA and LCCA.
- Task 3: Assess the sustainability of novel combined cation-anion exchange (CCAE) systems and compare them to conventional systems.

- Task 4: Disseminate results of research among stakeholders, develop a simplified tool for evaluating and comparing sustainability of IX system designs that can be used by the water professionals, and contribute toward development of a sustainability assessment framework that takes into account their feedback.

1.1 Intellectual Merit

This research advances the understanding of IX technology by using a life cycle approach to evaluate environmental and economic sustainability. It also develops a novel method for assessing and improving the sustainability of IX by tightly integrating process models with LCA/LCCA. The computer model developed through this approach can be expanded upon by the academic community. As further studies are performed on the sustainability of IX systems, new results can be added to the model in a modular fashion, increasing its impact, longevity, and value to the academic community. Furthermore, industry contacts have expressed interest in applying the model developed. Therefore, the simplified design tool will allow for the drinking water community and IX industry to apply the research results in order to identify improved system designs. This research also promotes the role of a life cycle sustainability approach in technology development, which assists in avoiding shifting of environmental and economic impacts from one phase of the life cycle to another.

1.2 Broader Impacts

This research not only provides a significant step forward in understanding the environmental and economic costs of IX systems, but translates this understanding into methods and tools for technology development that are appropriate for use in both academic and industry settings. Task 4 of this research further engages practitioners in the drinking water community through direct communication of results and use of feedback to develop tools for technology improvement that can be implemented in the field. Furthermore, this research complements other research on sustainability and the water-energy nexus at the University of South Florida (USF) and is developing mutually beneficial research relationships between USF and University of Florida (UF). This research is producing publishable results that are being presented at conferences to engage both the academic and practitioner community.

1.3 References

Ali, I., Gupta, V. K. (2007). Advances in Water Treatment by Adsorption Technology. Nature Protocols. 1, 2661-2667.

Andrews, D., & Harward, C. (1994). Isleham Ion-Exchange Nitrate-Removal Plant. Water and Environment Journal Water & Environment J, 120-127.

Argyris, C., & Schon, D. (1974). Theory in practice: Increasing professional effectiveness. San Francisco: Jossey-Bass.

Azapagic, A. (1999). Life cycle assessment and its application to process selection, design and optimisation. Chemical Engineering Journal, 1-21.

Azapagic, A., Millington, A., & Collett, A., 2006. A Methodology for Integrating Sustainability Considerations into Process Design. *Chemical Engineering Research and Design, 84*(6), 439-452. doi:10.1205/cherd05007

Bansal, P., Bertels, S., Ewart, T., Macconnachie, P., & O'brien, J. (2012). Bridging the Research-Practice Gap. Academy of Management Perspectives, 73-92.

Bero, L., Grilli, R., Grimshaw, J., Harvey, E., Oxman, A., & Thomson, M. (1998). Getting research findings into practice: Closing the gap between research and practice: An overview of systematic reviews of interventions to promote the implementation of research findings. BMJ, 465-468.

Choe, J.K., Mehnert, M., Guest, J., Strathmann, T.J., Werth, C.J., 2013. Comparative assessment of the environmental sustainability of existing and emerging perchlorate treatment technologies for drinking water. Environ. Sci. Technol. 47, 4644-4652.

Choe, J., Bergquist, A., Jeong, S., Guest, J., Werth, C., & Strathmann, T. (2015). Performance and life cycle environmental benefits of recycling spent ion exchange brines by catalytic treatment of nitrate. Water Research, 267-280.

Clifford, D., Lin, C., Horng, L., and Boegel. J. (1987). Nitrate removal from drinking water in Glendale, Arizona. EPAl600152-861107. U.S. Environmental Protection Agency (EPA). Cincinnati. Ohio.

Dahab, M. (1987). Treatment Alternatives for Nitrate Contaminated Groundwater Supplies. Journal of Environmental Systems, 65-75.

Dominguez-Ramos, A., Chavan, K., García, V., Jimeno, G., Albo, J., Marathe, K.V., Yadav, G.D., Irabien, A., 2014. Arsenic removal from natural waters by adsorption or ion exchange: an environmental sustainability assessment. Ind. Eng. Chem. Res. 53, 18920-18927.

European Environment Agency, (2012). Towards Efficient Use of Water Resources in Europe. Copenhagen.

Fazeni, K., Lindorfer, J., & Prammer, H., 2014. Methodological advancements in Life Cycle Process Design: A preliminary outlook. *Resources, Conservation and Recycling, 92*, 66-77. doi:10.1016/j.resconrec.2014.08.011

Kapoor, A., & Viraraghavan, T. (1997). Nitrate Removal From Drinking Water—Review. Journal of Environmental Engineering J. Environ. Eng., 371-380.

Langrall, C. (2014). Linking Research and Practice: Another Call to Action? Journal for Research in Mathematics Education, 45(2), 154-156.

Maul, G., Kim, Y., Amini, A., Zhang, Q., Boyer, T., (2014). Efficiency and Life Cycle Environmental Impacts of Ion-exchange Regeneration Using Sodium, Potassium, Chloride, and Bicarbonate Salts. Chemical Engineering Journal. 254, 198-209.

Panswad, T., Anan, C., (1999). Impact of High Chloride Wastewater on an Anaerobic/anoxic/aerobic process with and without Inoculation of Chloride Acclimated Seeds. Water Research. 33, 1165-1172.

Ras, C., von Blottnitz, H., (2012). A comparative life cycle assessment of process water treatment technologies at the Secunda industrial complex, South Africa. Water SA. 38, 549-554.

Richard, Y. (1989). Operating Experiences of Full-Scale Biological and Ion-Exchange Denitrification Plants in France. Water and Environment Journal Water & Environment J, 154-167.

Rogalla, F., Ravarini, P., Larminat, G., & Couttelle, J. (1990). Large-Scale Biological Nitrate and Ammonia Removal. Water and Environment Journal Water & Environment J, 319-328.

United Nations Environment Programme and International Water Management Institute. (2012). Ecosystems for Water and Food Security. Nairobi and Colombo.

United States Environmental Protection Agency (USEPA). (2013). 2013 National Public Water Systems Compliance Report (EPA DOCUMENT 305R15001).Washington, DC: Office of Enforcement and Compliance Assurance (2201A).

Vorosmarty, C. J., Green, P., Salisbury, J., & Lammers, R. (2000). Global Water Resources: Vulnerability from Climate Change and Population Growth. Science, 289(5477), 284-288. doi:10.1126/science.289.5477.284

Chapter 2: Environmental and Economic Sustainability of Ion Exchange Drinking Water Treatment for Organics Removal [1] (Task 1)

2.1 Abstract

Water treatment infrastructure faces numerous operational and financial challenges in most regions of the world. Ion exchange is a water treatment technology that can be used to remove various contaminants in drinking water and has shown increased adoption in recent years due to its operational advantages; however, limited research has been conducted on the environmental and economic sustainability of ion exchange systems. This study utilizes life cycle assessment and cost analysis to holistically evaluate environmental and economic impacts of ion exchange technology that is used for reduction of disinfection by-products via organics removal in eight drinking water treatment plants in Florida. A functional unit accounting for both water quantity and quality was used and showed to have a significant effect on the evaluation results. Impact assessment results show that the construction phase has negligible environmental impact in comparison to the operation phase. Systems that use fixed bed reactors with conventional resin were compared with systems using completely mixed flow reactors with magnetic ion exchange resin. Fixed bed systems evaluated have higher salt usage and brine waste production, but use less electricity, resin, and require less transport of materials. This

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tradeoff causes fixed bed systems to have a higher environmental impact in categories of eutrophication, carcinogenics, non-carcinogenics, and ecotoxicity but lower impact in other categories. Furthermore, it causes fixed bed systems to have a lower operation cost compared with completely mixed systems. Results also show that both environmental impacts and operation costs per functional unit decrease with scale, similar to economies of scale effects.

2.2 Introduction

Potable water systems face numerous environmental and economic challenges in most regions of the world and in 2012 approximately one fourth of all potable water systems in the U.S. were in significant violation of EPA or state rules (USEPA, 2012). Constant increases in water demand as well as improved understanding of environmental impacts associated with water treatment further highlights the need for economically and environmentally sustainable water treatment technologies (European Environment Agency, 2012; UNEP and IWMI, 2012). Ion exchange (IX) is a type of technology that can be used to remove hardness and a wide range of contaminants from drinking water, such as nitrate (Clifford & Liu, 1993), perchlorate (Urbansky, 2002), arsenic (Ghurye et al., 1999), bromide, dissolved organic carbon (DOC) (Hsu and Singer, 2010), cobalt (Rengaraj and Moon, 2002), and uranium (Gu et al., 2005). In terms of technical performance, IX is an effective and robust technology that can perform under varying water chemistry to meet the required water quality. From an operational standpoint, IX is flexible in terms of operation mode, reactor configurations, and sequence in a treatment train. Considering implementation, IX is a scalable technology that can be employed in centralized treatment systems as well as decentralized systems, such as household treatment. Therefore, IX provides a variety of advantages that offers opportunities for safe, affordable, and appropriate potable water treatment.

Implementation of IX systems, however, introduces environmental and economic burdens due to the energy and materials used in their construction and operation. Furthermore, disposal of waste brine produced in the resin regeneration process can have a variety of negative environmental implications. Waste brine with high salinity that is sent to wastewater treatment plants can affect their operation, particularly when biological processes are used (Maul et al., 2014; Panswad and Anan, 1999). Furthermore, discharge of wastes with high NaCl concentrations to receiving waters can have adverse effects on those ecosystems (Canedo-Arguelles, 2013). As the use of IX for drinking water treatment becomes more prominent (Ali and Gupta, 2007), understanding the environmental and economic consequences of their construction and operation becomes essential.

A variety of past studies have investigated the operation and performance of IX systems (Clifford et al., 2011), yet few studies have investigated the environmental and economic impacts of IX technologies over the life cycle. Life cycle assessment (LCA) is a method of quantifying environmental impacts of systems and can be applied as a useful tool for assessing the environmental sustainability of water treatment technology. LCA has been used to assess impacts of IX for perchlorate removal from drinking water and suggests that the regeneration process can be the most significant contributor to environmental impact of IX technologies (Choe et al, 2013). This is most likely because perchlorate has a high affinity for IX resin, therefore requiring large quantities of NaCl and producing large volumes of brine waste that require treatment or disposal. LCA studies have also been conducted to investigate how IX is comparable to other treatment technologies. For example, IX was found to have better environmental performance in impact categories of abiotic resource depletion and greenhouse gas emissions because of its low electricity requirements, but was not preferable in the categories of human toxicity and freshwater aquatic ecotoxicity compared with reverse osmosis (RO) for water softening (Ras and von Blottnitz, 2012). Comparison of selective IX (without regeneration) to biological reduction of perchlorate with acetate as well as catalytic reduction processes for perchlorate treatment revealed that IX is a better choice than the other two alternatives, which have high impacts associated with electron donor production (acetate) and catalysts such as palladium and rhenium (Choe et al, 2013). However, an alternative electron donor was not investigated in that study, which could potentially reduce impacts. Furthermore, use of IX for removal of arsenic from drinking water was found to consume up to 13 times less primary resource and 17 times less environmental burdens than adsorption of arsenic (Dominguez et al., 2014).

These results, however, are likely to be context and design sensitive and may therefore vary for IX systems that treat other contaminants or use alternative designs. In recent years, due to heightened disinfection by-product (DBP) regulations, IX treatment has become a favored method of DOC removal for DBP reduction in many regions. However, no studies have investigated the sustainability of IX for organics removal. Moreover, no studies have investigated the influence of system designs (e.g. reactor configurations, scale) on environmental impact and cost of IX systems. Different reactor configurations can result in significant differences in the amount and type of resin used, the amount of salt required, and the volume of waste brine generated. Potential differences in scale also hold important implications for how LCA studies are carried out. For example, when selecting a product for the life cycle inventory, one would also need to consider at what scale it was manufactured. The impact of scale, however, has often been neglected in environmental impact assessments (Lundin et al., 2000). Moreover, previous studies only consider one IX treatment plant, whereas differences in management practices and operator training can significantly affect operation. Therefore, evaluation of a larger number of IX plants with different reactor configurations and scales is necessary to obtain a sound understanding of environmental sustainability of IX technology.

In addition to environmental sustainability, it is necessary to ensure cost effectiveness of IX technologies. The few studies that have evaluated IX costs seem to suggest that for perchlorate removal the industry has moved toward using selective IX due to its lower cost (Choe et al., 2013). For selective IX systems, resin is used until saturation and replaced with new resin; the used resin is either incinerated or disposed in a landfill. Using a selective IX system for perchlorate is beneficial because perchlorate regeneration requires extremely large amounts of salt. This is likely to differ for IX systems that remove organics; however, studies on cost analysis of other IX systems are extremely rare. Increased understanding of the cost tradeoffs of IX systems is needed to balance economic and environmental concerns.

The purpose of this study is to assess environmental and economic impacts of IX systems that are implemented to reduce DBP formation in drinking water by removal of organics. This study uses a life cycle approach to evaluate the relative contribution of construction and operation phases of IX systems, identify the primary contributors of operation impacts, compare competing reactor designs and material choices, and examine the relationship between scale and environmental and economic burdens. Furthermore, the advantages of choosing a functional unit that takes into account water quality, as well as quantity, is discussed and presented.

2.2 Materials and Methods

The study follows International Organization for Standardization (ISO) methodological framework for environmental impact assessment, including Goal and Scope Definition, Inventory Analysis, Impact Assessment, and Interpretation (ISO, 2006a; ISO, 2006b).

2.2.1 Goal and Scope

This study is intended to provide an understanding for both industry and academic audiences of the environmental impacts and costs of IX technologies currently in operation for organics removal. From an industry perspective, this understanding can help to improve the environmental and economic sustainability of IX systems through better design, training, and operation. From an academic perspective the assessment results can be used to develop models incorporating the sustainability of IX systems. Furthermore, it provides a baseline of comparison to ensure that IX technology improvements do not shift burdens from one area in the life cycle to another.

2.2.1.1 Functional Unit Selection

The function of the systems in this study is to remove organic carbon from water. Therefore, the functional unit (FU) chosen was 1 million gallons (MG) of water treated with 1 mg/L DOC removal over the course of 20 years. A 20 year timescale was used because it is the design life for most of the plants studied. In water treatment systems, often a FU is chosen that only takes into account water quantity treated (Barrios et al., 2008; Vince et al., 2008); however, the function of water treatment systems is not only to process a quantity of water, but to improve the water quality to the standard. A system may be designed to process large quantities of water, but if it cannot remove contaminants efficiently, additional infrastructure, materials, and processes will be required. Therefore, taking into account water quality in the FU provides a more fair comparison of systems based on their ability to achieve the desired function. A comparison of the results based on an FU that incorporates water quality and quantity as opposed to the conventional method of using water quantity alone, is presented in section 3.2.2 to demonstrate the advantages and disadvantages of each method.

In order to create a FU that incorporates water quality, a common treatment parameter for organic carbon must be measured at the influent and effluent of the IX units. Approximately half of the plants in the study monitored the organic carbon by measuring color while the others measure UV absorbance (UVA254). While these measurements are easier to perform at the treatment plant, DOC provides a more direct measurement of organics. Therefore, all influent and effluent organics concentrations were converted to an estimate of organic carbon, measured as DOC. The relationship between color, UVA254, and DOC can vary, depending on water sources. Therefore, influent and effluent samples were taken from a majority of the treatment plants and the three parameters were measured in all the samples. This was used to create a regression equation describing the relationship between the three parameters for Florida groundwater, which was used to estimate the influent and effluent DOC concentrations in the plants that could not be directly sampled. The regression equations are included in the Supplementary Information (SI) (Figures 2.8-2.9).

2.2.1.2 System Boundary

The system boundary used in this study includes raw material extraction, production, transportation, construction, operation, and use of recovered materials and energy. Construction of significant infrastructure is included but decommission of that infrastructure is not. A diagram of the system boundary, including upstream processes, IX system operation, and downstream processes, is shown in Figure 2.1.

Within the context of a drinking water treatment plant, the system boundary of this study only includes the systems necessary to carry out the IX process. Therefore, any pretreatment before IX, such as lime softening, and any post-treatment, such as disinfection, that are not necessary for IX operation were not included in this assessment. However, the water quality portion of the functional unit takes into account any differences in water quality at the influent and effluent of the IX process that may be due to differences in pretreatment.

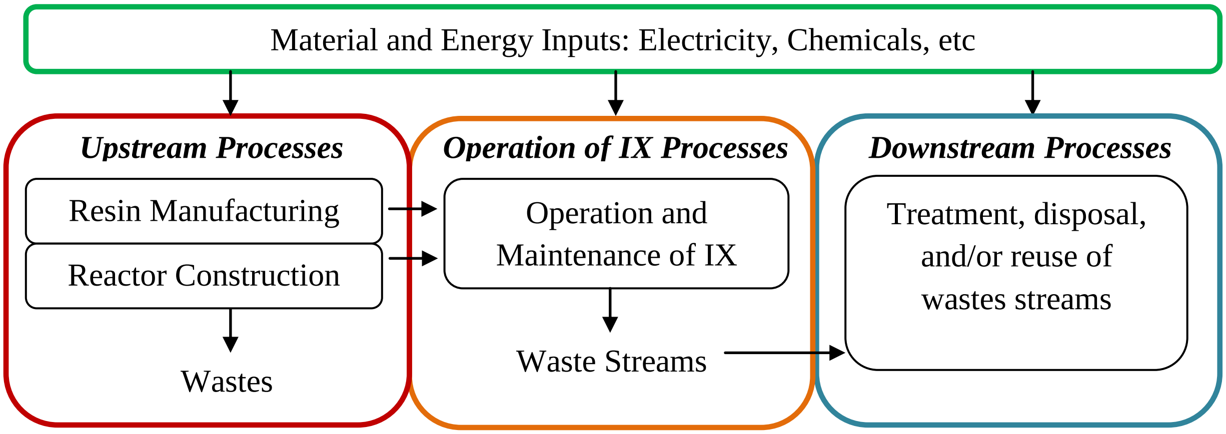

Figure 2.1: The system boundary of the life cycle assessment of ion exchange process in the study includes upstream and downstream processes as well as operation

2.2.2 System Descriptions

Data that was used for the life cycle inventory was collected from eight drinking water treatment plants in Florida that use IX technology. All of the plants used IX to remove organic carbon to prevent formation of DBPs. Two of the plants also used IX to remove hardness from the water; however, these systems were not evaluated in this study. Groundwater is the water source for all of the plants that were found to employ IX in Florida and the average flow rates ranged from 0.078-8.5 million gallons per day (MGD). The plants included in the study were chosen because they are considered by the authors to be representative of the IX drinking water plants in Florida and include a range of scales, as measured by average flow rate. Table 2.1 shows the plants included in this study, along with pertinent information about each plant. Flow diagrams of each plant are provided in the SI (Figures 2.10-2.15).

The plants generally fall into two categories: those that use magnetic ion exchange (MIEX) resin and those that use conventional resin. The conventional resin is a polystyrene strong base type anionic resin, A-72MP (Thermax Tulsion, Pune, India). The MIEX resin is a proprietary magnetically enhanced anionic polyacrylic resin (Orica Watercare, Melbourne, Australia). All of the MIEX systems employ a completely mixed flow reactor (CMFR), whereas the systems with conventional resin use fixed bed reactors (FBR). These differences in design create significant differences in the construction and operation of these systems that are reflected in the environmental impact and cost assessment results.

Table 2.1: Eight drinking water treatment plants were included in this study and important characteristics were categorized such as include flow rate, influent/effluent concentrations, and reactor type.

Plant Studied:	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**
Flow Rate Capacity (MGD)	10	4	4	9	1	1.44	0.4	0.5
Estimated Average Flow Rate (MGD)	8.5	2.6	1.9	4.5	0.45	0.33	0.2	0.078
Estimated Average Influent DOC (mg/L)	8.1	6.47	9.21	3.61	5.97	4.79	3.45	3.08
Estimated Average Effluent DOC (mg/L)	1.6	2.33	2.48	0.66	1.59	4.47	2.12	1.53
Reactor Type	Fixed Bed	Fixed Bed	Fixed Bed	CMFR	CMFR	CMFR	CMFR	CMFR
Year Built	2008	2008	2004	2008	2011	2008	2009	2011

Data collected for average flow rates and average influent/effluent concentrations are considered to be representative of typical conditions. These data were collected by evaluating recorded plant operation data, consulting with plant operators, and direct sampling. The treatment plants had influent DOC concentrations of approximately 3-9 mg/L with effluent concentrations ranging from approximately 0.7 to almost 5 mg/L. The plants evaluated within this study have all been built within the past 10 years, which reflects the recent increased adoption of IX technology for removal of organics in drinking water.

2.2.3 Life Cycle Inventory Methods

An inventory of materials and energy was developed for all of the plants, based on data collected through plant visits and evaluations, conversations with plant operators, information provided by the engineering designers, and information provided in the system manuals. An inventory was generated for both construction and operation phases for one FBR system and one CMFR system (Plants A and G). This was used to investigate the relative contribution from construction and operation phases to the overall impacts. For the remaining plants, only inventory data on the operation phase was collected. This made inventory data collection more feasible, allowing for a larger sample of plants to be evaluated.

Foreground data, meaning the inventory data specific to the system studied, include the construction materials, salt usage, brine waste production, resin usage, electricity usage, and other chemical requirements such as hydrochloric acid or sodium hydroxide. However, background data, meaning generic or average data typically found in databases or literature, were obtained from Ecoinvent 3 and USLCI databases, available in Simapro version 8.0.3. In some cases economic input-out data was used when detailed material information was not available. In cases where specific materials were unavailable from the databases, new processes were created to closely estimate the actual product in order to determine if it was significantly different from the data available in the database. For example, anionic resin available in Ecoinvent 3 database uses polystyrene resin, like the conventional resin; however, the MIEX resin is made of polyacrylic. Therefore, a new process was created for MIEX resin using polyacrylic to observe potential differences between the two materials. However, differences between them were negligible and therefore the standard anionic resin was used in the assessment.

2.2.4 Life Cycle Impact Assessment Methods

The life cycle impact assessment (LCIA) was performed using the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI 2.1) (Bare et al., 2003), which was chosen because it utilizes assessment methods suitable for North America. The impact categories include: ozone depletion, global warming, acidification, eutrophication, eco-toxicity, smog formation, human health carcinogenics, human health non-carcinogenics, human health criteria pollutants, and fossil fuel use.

Although the TRACI methodology does not generally aggregate between environmental impact categories, in this assessment characterization results were aggregated in some cases to obtain a single score. This allows for a clear comparison among water treatment plants. To obtain a single score, the results were normalized using normalization values found in Bare et al. (2006) and aggregated using an equal weighting among all categories. Weighting among categories in LCA assessments is considered a subjective process and will vary depending on the context and audience of the LCA assessment. Equal weighting is used in this assessment to reduce possible uncertainty due to subjective judgments and provide an evaluation that is typical for the systems studied. Furthermore, audiences with specific interests can use the data included in the SI to perform weighting for a particular context.

2.2.5 Life Cycle Operation Cost Analysis

A cost analysis was performed on the same systems evaluated in the LCA. Due to limitations in data availability and confidentiality, capital costs were not able to be directly collected for most of the plants. However, a simple capital cost comparison between the two types of systems is included. Operating expenses (OPEX) were collected and calculated using information from the plant operators, managers, and engineering manufacturers. Cost of labor was also not included in the scope of the analysis. Furthermore, the cost of salt and resin includes the cost of transport. All cost calculation results are presented in 2014 dollars.

The OPEX was calculated using present value method by multiplying annual operating costs by a uniform present value (UPV) factor. The UPV was calculated using Equation 1, with an interest rate (i) of 5% for a lifetime (n) of 20 years. Using a UPV assumes that the annual operating costs are constant in the study period. For energy cost, a non-uniform present value (UPV*) was calculated using Equation 2. The Energy Efficiency and Renewable Energy (EERC) program (version 2.0-13) from the U.S. Department of Energy was used to calculate the annual energy escalation rate (e) of 0.65% for Florida, with a default carbon price.

$$\text{UPV factor}= \frac{(1-(1+\mathrm{i})^{-\mathrm{n}})}{\mathrm{I}} = \frac{\left(1-(1+0.05)^{-20}\right)}{0.05} = 12.46 \qquad (1)$$

$$\text{UPV* factor}= \frac{(1+e)}{(i-e)}\left[1-\left(\frac{1+\mathrm{e}}{1+\mathrm{i}}\right)^{\mathrm{n}}\right] = \frac{(1+0.0065)}{(0.05-0.0065)}\left[1-\left(\frac{1+0.0065}{1+0.05}\right)^{20}\right] = 13.21 \qquad (2)$$

2.2.6 Data Quality

The data used in this study was collected from a variety of sources including plant managers and operators, engineering manufacturers, contractors, system manuals, engineering drawings, municipal budgets, and direct measurement. Effort was also made to verify information through multiple sources. For example, information gleaned from systems manuals regarding resin addition requirements were verified with plant operators to ensure that these were the procedures they followed.

The geographic coverage of the data is limited to Florida. Assumptions made in the life cycle inventory are provided in the SI (Table 2.2). The data on water quantity and quality was provided by plant managers and operators, plant logs, and water quality tests. In some cases, long term data was unavailable for influent/effluent concentrations and seasonal or weather fluctuations can potentially change these concentrations throughout the year. For the purpose of a comparative assessment, however, the data was collected under the same conditions for consistency.

2.2.7 Analytical Methods

As described in section 2.2.1.1, influent and effluent samples were taken at several treatment plants to determine the DOC concentration. This was utilized with existing data on the UV absorbance (UV_{254}) and Color to generate a regression equation that estimates the relationship between the three parameters. This relationship can vary depending on a number of source water characteristics; therefore, the regression equation is expected to be accurate mainly for Florida groundwater sources. All experiments were conducted in triplicate and samples were filtered through 0.45 μm nylon membrane filters (Millipore) prior to the analysis. All filters were pre-rinsed with 500 mL of DI water followed by 10 mL of sample. DOC was analyzed by combustion with a total organic carbon analyzer (Shimadzu, TOC-V_{CPH}) with an ASI-V autosampler. All of the samples were run in duplicates on each instrument. Standard calibration checks for the total organic carbon analyzer were within 10% of the known value.

2.3 Results and Discussion

2.3.1 Life Cycle Inventory

A construction phase inventory was compiled for two of the plants in order to provide a representative evaluation of the significance of the construction phase as compared to the operation phase. The main components of the construction inventory include materials for tanks and vessels, pumps, agitators, and piping. Tanks and vessels account for the majority of the total mass of materials required. In CMFR systems, tanks and vessels account for approximately 60% of the total mass, while agitators and control panels each account for about 20% of the total mass. FBR systems, however, do not require agitation; therefore, tanks and vessels account for over 80% of the total mass input, with large pumps also being a significant portion of the input. A detailed construction inventory is located in the SI (Tables 2.3-2.4).

An inventory of energy and materials used in the operation phase was compiled for all of the plants. The main components generally include: electricity usage, regenerant salt usage, brine waste treatment or disposal, resin addition, transport, and in some cases acid or base addition. Regular addition of virgin resin is necessary for the CMFR plants due to the consistent loss of MIEX resin during operation. These MIEX resins break down over time and exit the reactor. They are expected to be caught by sand filters further down in the treatment train or by magnetic polishers designed to capture the resins. In some cases, acids such as HCl were added for the purposes of cleaning or maintaining MIEX resins that became fouled. In most cases, only periodic cleaning was required, but in some cases weekly addition of acids was employed to ensure fouling of the resin did not occur due to high iron concentrations in the source water.

The conventional resins also require eventual replacement; however, replacement of conventional resin is done in a non-continuous fashion, only after significant fouling has occurred to the point where replacement would be economically beneficial. Fouling of the resins reduces ion exchange capacity and causes more frequent regenerations to be required. The lifetime of the conventional resin can vary depending on operation of the system. This is because operator choices, such as how pH is controlled when IX is implemented after lime softening, can increase or decrease fouling. Furthermore, operators can implement periodic deep cleaning of the conventional resin, often using a caustic such as NaOH, to reduce fouling and regain IX capacity. In this assessment, a conservative estimate of 15 years for lifetime of the conventional resins was used, based on conversations with IX system manufacturers. A detailed inventory of the operation phase for each plant is located in the SI (Table 2.5).

The inputs during operation also show tradeoffs between FBR and CMFR systems. A normalized comparison between the main inputs for both systems is shown in Figure 2.2. FBR systems have lower electricity usage, resin addition, and transport requirements (measured in ton*km or tkm) while CMFR systems have much lower salt requirements and brine waste production. These tradeoffs are directly tied to differences in design of these systems. Because the CMFR systems continually lose resin, virgin resin must be purchased regularly. This requires large amounts of the proprietary MIEX resin. The FBR systems are not considered to lose resin regularly, but do require eventual resin replacement. The total resin requirements for FBR systems, however, are a fraction of those required for CMFR systems. The main transport requirements are for salt and resin. The high amount of resin required for CMFR systems as well as their long transport distance (from Australia) results in higher overall transport requirements compared with FBR systems.

The salt usage, brine waste generated, and transport requirements are all directly tied to regeneration requirements of the systems. To regenerate IX resin, a highly concentrated brine solution is needed, often using NaCl salt. This requires large masses of salt to be manufactured and shipped to the plant location. After the regeneration process is complete, the brine contains high concentrations of organics and must be treated or disposed of. For most of the systems, brine waste was disposed of by dilution and slow discharge to the wastewater treatment plant (WWTP). Most of the plants used extremely concentrated brines. Using lower brine concentrations can be just as effective, allowing for lower salt usage, but this may require longer regenerations, more water use, and more control/monitoring of the brine by operators. None of the plants in this study employed methods to remove organics from the brine to allow for brine reuse, but some treatment plants recovered a portion of the brine that had low conductivity and

DOC and sent it back to the head of the plant. Some plants also monitored conductivity of the brine and reused it until it dropped below a threshold. Implementation of full or partial brine reuse could not only reduce the amount of brine waste that requires disposal, but could also significantly reduce both salt manufacturing and transport requirements, decreasing costs and environmental impacts significantly.

In addition to brine reuse, another means of reducing salt usage, brine production, and transport is to reduce the number of regenerations required. In theory, FBR systems which implement a plug flow design, should use less salt due to better efficiency than a CMFR design. However, the opposite was found to be true. This is likely because one of the main influences on regeneration requirements is resin capacity, which can decrease as resin ages and resin fouling occurs. In CFMR systems, where new resin is continually added, upkeep of the resin is less of a concern. In FBR systems, however, the resin can last for long periods of time and lack of proper maintenance of the resins can cause increased need for regenerations. For example, the FBR systems evaluated in this study employ similar designs, but Plants B and C regenerate the resin for every 2 million gallons of water treated, whereas Plant A is able to regenerate for every 7 million gallons of water treated. Therefore, Plant A requires less salt, less transport, and produces less waste. The superior performance of Plant A may be attributed to excellent management and operator training as well as data collection. Very few of the treatment plants monitored their system closely and even fewer kept significant records. Plant A, however, kept detailed records of the plant operation and regularly implemented caustic resin cleans, to maintain high IX capacity and increase cost effectiveness of the resin.

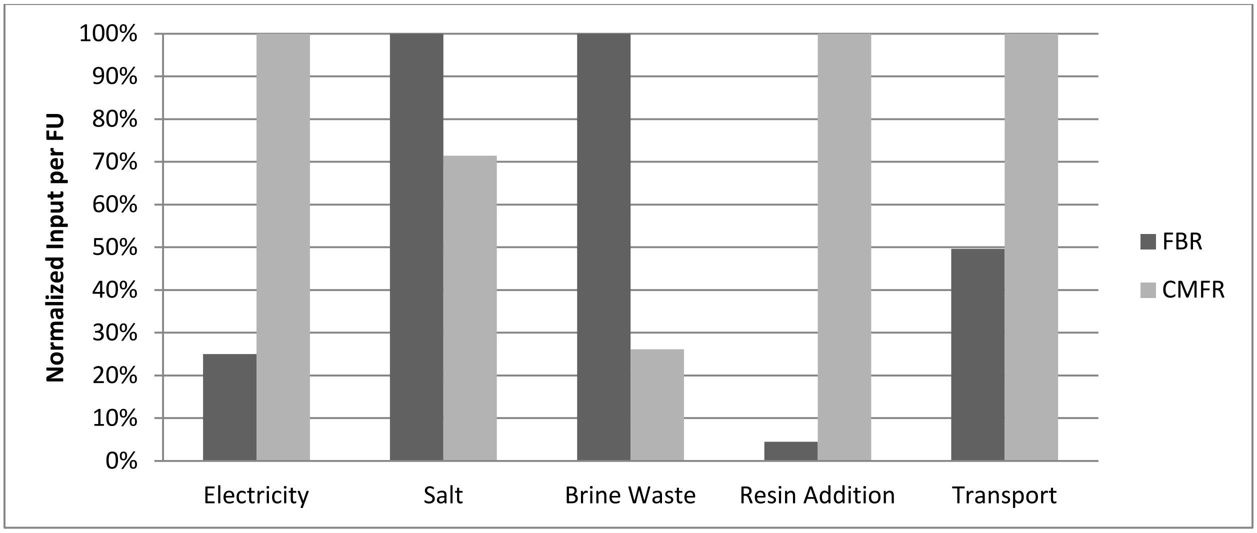

Figure 2.2: Normalized comparison of the main inputs for fixed bed reactor (FBR) and completely mixed flow reactor (CMFR) systems shows that FBR systems have lower requirement on electricity, resin addition, and transport, but use more salt and produce more brine waste than CMFR systems.

The electricity consumption is lower in FBR systems. The main electricity consumer in FBR systems is the pumping required for moving water through the treatment system as well as to perform backwashes and brine regeneration. CMFR systems, however, also require electricity for mixing in the contactor as well as regeneration tanks. This is either achieved by agitation or pump mixing. Therefore, a possible means of reducing electricity consumption in the CMFR systems could be to employ methods of passive mixing that do not require electricity input.

2.3.2 Impact Assessment

2.3.2.1 Operation vs. Construction

To understand the relative importance of environmental impacts due to the construction phase vs. impacts due to the operation phase, both were assessed for one FBR and one CMFR plant. Plants A and G were used in this assessment because a large amount of data was available for both plants and their construction materials and processes are considered by the authors to be representative of properly maintained IX plants. Plant A uses a FBR reactor design for IX with a lifetime of approximately 30 years, while Plant G uses a CMFR design with a lifetime of approximately 20 years.

The impact assessment results for the two systems, shown in Figure 2.3, are normalized to show the percentage of total impact from each phase. The results show that in both systems, the impacts due to operation significantly outweigh construction in all categories. The impacts due to the construction phase are generally less than 10% of the total impacts, except for impact categories of eutrophication, carcinogenics, non-carcinogenics, and ecotoxicity for Plant G, where the construction phase contributes 20-30% of impacts. This is mainly due to the treatment of sulfidic tailings required during the production of the electronics used in the control panels. In Plant A, the main exceptions are in the carcinogenic and ecotoxicity impacts, where the construction phase contributes approximately 25% and 20%, respectively. This is due to the reinforcing steel used in the large pumps and IX vessels of the plant. Although in some categories the construction phase can contribution significantly, in most categories the operation phase dominates the total environmental impact. Furthermore, collection of the construction phase inventory for a large number of plants was not feasible. Moreover, neglecting the contribution of construction still allows for a fair comparison between treatment plants. Therefore, it is assumed that impacts from construction phase can be neglected in the rest of the study. This assumption is further supported by the work of previous researches (Choe et al, 2013). Therefore, in the following sections the remaining plants are assessed and compared by the operation phase alone.

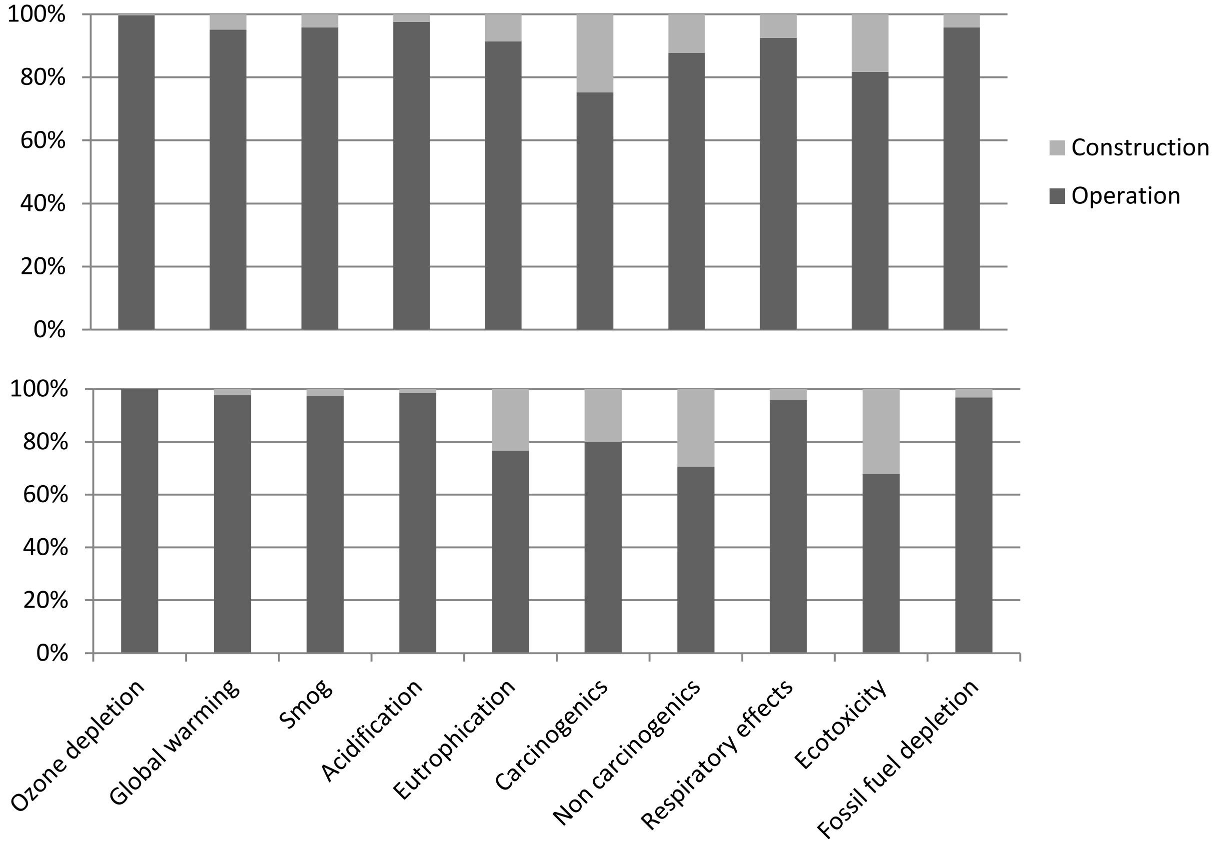

Figure 2.3: A normalized impact assessment of construction versus operation for plant A (above), which uses a fixed bed reactor (FBR), and plant G (below), which uses a completely mixed flow reactor (CMFR), shows that the construction phase is relatively negligible.

2.3.2.2 Comparison of Functional Unit Choice

The FU selection can have significant effects on the impact assessment results. An aggregated single score of environmental impacts was calculated for each plant and normalized using flow rate alone and flow rate with DOC removal, as shown in Figure 2.4. Taking into account water quality significantly alters the relative impact between the plants. For example, Plant C has higher environmental impacts compared with Plant B when only water quantity is taken into account; however, when both quantity and quality are measured, its impact becomes lower than Plant B due to higher removal efficiency. Furthermore, based on quantity alone, Plants E and H have higher impacts than G, but when quality is accounted for, their impacts become less. In other cases, such as Plant F, the impact increases significantly compared to the other treatment plants.

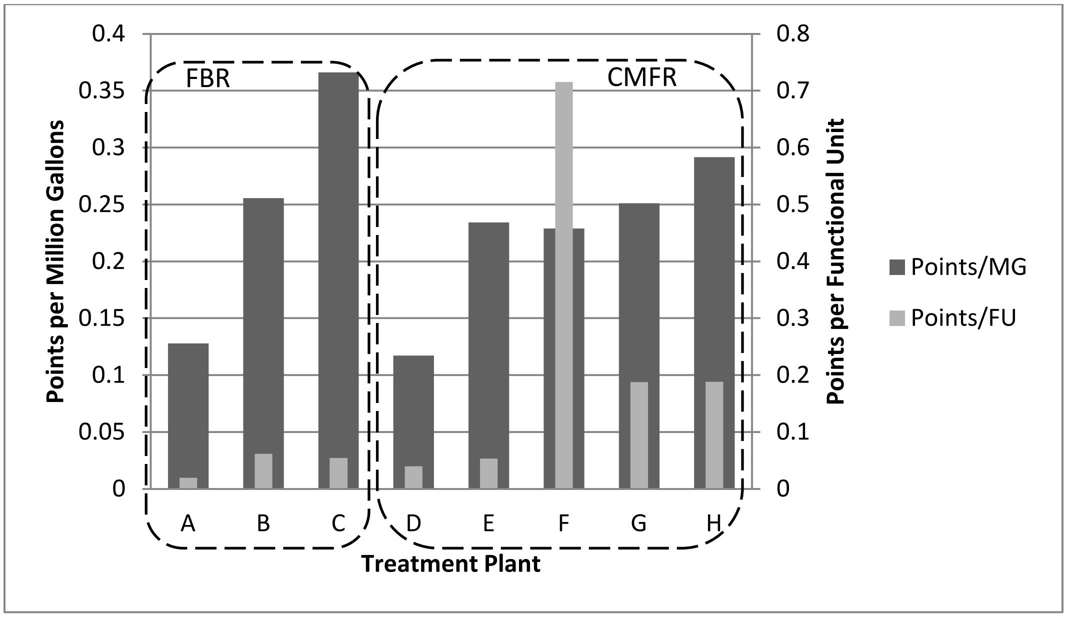

Figure 2.4: A single score comparison of environmental impacts of the operation phase of the water treatment plants, normalized by flow rate in million gallons (MG) and water quality in dissolved organic carbon (DOC) (mg/L), shows the differences between the individual plants and system types.

The high impact of Plant F is mainly attributed to the extremely low contaminant removal achieved. It demonstrates importance of ensuring that IX systems are functioning at high removal ability. Furthermore, in some cases where influent concentrations may already be very low, high removal is not possible, highlighting the importance or ensuring that conditions merit installation of a complex water treatment system. For example, locations that have influent DOC concentrations of 6-9 mg/L would be preferable because they allow for high organics removal, thereby decreasing the overall impact per functional unit. If concentrations of the raw water are low in a particular location, an alternative and simpler technology may be preferable. The organics removal of Plant F are not considered by the authors to be representative of MEIX systems and the plant does not have a record of influent and effluent DOC concentrations;

therefore, it is excluded in the following environmental impact analyses in order not to skew results.

2.3.2.3 Operation Impacts

Plants A, B, and C all use an FBR design, while the others employ a CMFR design. Furthermore, the FBR plants have similar contaminant removal rates of 4-6 mg/L DOC. Differences, however, can still be seen among them, as shown in Figure 2.4. For example, plant A is shown to have lower impacts, and this is likely due to better maintenance of the resins by the operators, as discussed in section 2.3.1, which decrease regeneration requirements. This is done by ensuring resins have not been fouled and that the contactors have not lost resin volumes below design specifications. The main cause for variation in impacts among the CMFR plants, however, is more likely to be contaminant removal rates because some plants remove less than 1 mg/L DOC while others remove more than 4 mg/L.

2.3.2.4 Comparing Fixed Bed and CMFR Systems

The main impacts for FBR and CMFR systems were calculated and normalized, as shown in Figure 2.5. FBR systems have lower electricity usage, resin addition and transport requirements; however, they require more salt while generating more brine waste than the CMFR systems, as discussed in section 2.3.1. FBR systems tend to have higher impacts for the categories of eutrophication, carcinogenics, non-carcinogenics, and ecotoxicity because of the high impacts of salt production. However, CMFR systems have higher impacts in other categories, primarily due to resin production and electricity consumption. Recovery of the lost resin and employing passive mixing will help reduce environmental impacts associated with CMFR systems.

The impact of FBR systems is closely tied to regeneration frequency; therefore, the main reason the FBR systems show high environmental impacts is likely due to poor maintenance of resins, which increases regeneration frequency and salt requirements. Better maintenance of resins in the FBR plants is a key operational change required to reduce environmental impacts and could make them equal to or lower than those of CMFR plants in all categories. Therefore, although FBR systems have some clear advantages, if the resins are not maintained properly, they can be less environmentally friendly.

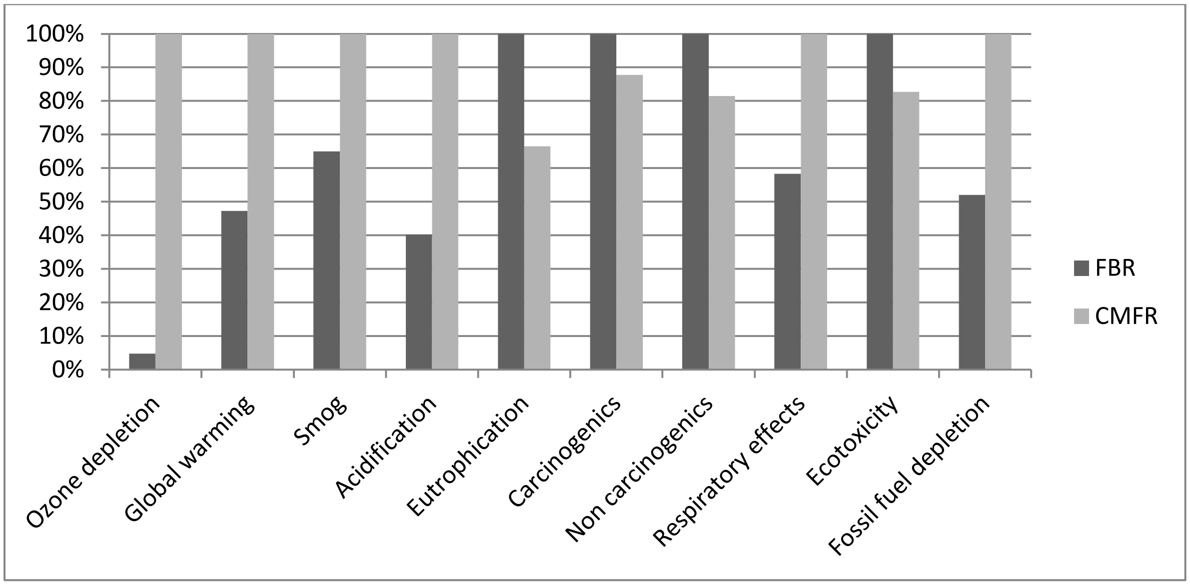

Figure 2.5: The average environmental impacts of fixed bed reactor (FBR) and completely mixed flow reactor (CMFR) systems show tradeoffs between the two types of systems.

Aside from resin maintenance, brine reuse can be employed in all system types to reduce the salt requirements. The high brine waste from FBR systems can also cause negative effects, which are not captured in the LCA results, on WWTP operation as well as within ecosystems to which WWTP effluent is discharged. Furthermore, in areas where WWTP effluent is used for irrigation, high brine concentrations can prevent agricultural use. In addition to reduction of brine wastes, alternative regenerants such as potassium or bicarbonate salts have been investigated as more environmentally friendly alternatives to NaCl when considering the impacts from brine disposal (Maul et al., 2014).

2.3.2.5 Effects of Scale

In most LCA models, environmental impacts are commonly assumed to increase linearly as scale increases (Curran, 2012). However, the impact assessment results indicate that at higher flow rates, the impacts per FU decrease, as shown in Figure 2.6. This seems to suggest that environmental impacts may follow a pattern similar to the principle of economies of scale. In some cases, the differences may be due to other factors, such as frequency of regeneration in FBR plants. To account for this, a test sample of data was evaluated with the regeneration frequency adjusted to be equal for all FBR plants. This caused a reduction in the difference between the plants, but the higher scale plants continued to show lower environmental impact. This may be due to more efficient use of pumping and mixing energy at larger scales, such as has been observed with other types of machines (Diaz et al., 2009). The results regarding the effects

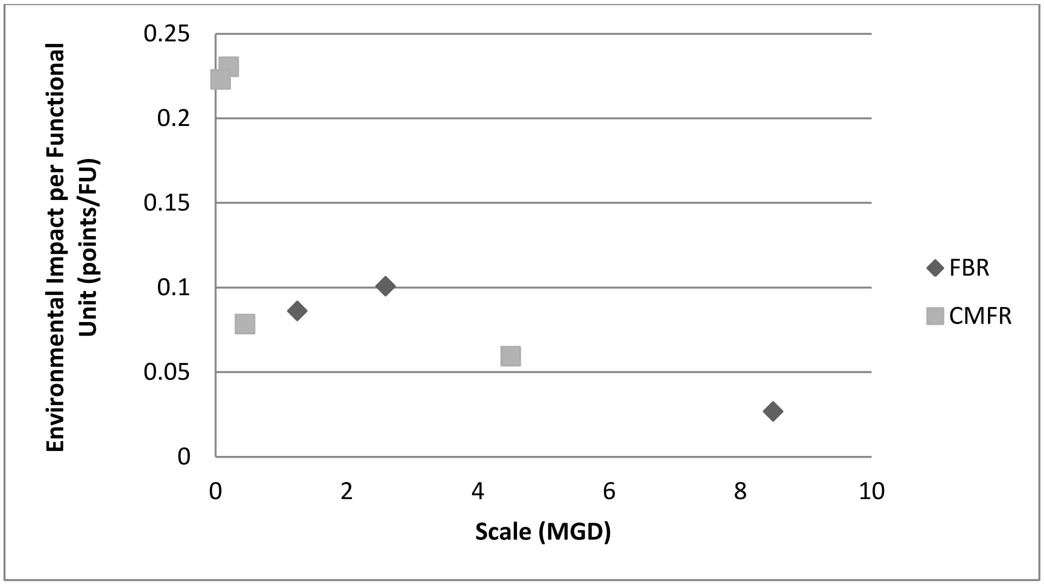

Figure 2.6: The relationship between environmental impact and scale for fixed bed reactor (FBR) and completely mixed flow reactor (CMFR) ion exchange systems shows a decrease in impact as scale increases.

of scale are based on a limited set of installations; therefore, a larger data set would allow for even more accurate estimation of a regression based on scale effects.

2.3.2.6 Cost Analysis Results

Costs of operation varied widely among the treatment plants. The most significant cost contributors were resin replacement, salt addition, electricity requirements, and acid/chemical addition. The lifetime operation cost per FU of the treatment plants was calculated and results show that the FBR plants have lower costs per FU than the CMFR plants. This is likely because the highest cost contributors in the FBR plants, such as salt and brine waste treatment, are relatively inexpensive. In most systems, brine waste was diluted and discharged at a slow rate to the WWTP, incurring negligible cost to the treatment plant. Bulk salt prices are also relatively low compared to high resin and electricity costs. Therefore, the relative importance of each of these contributors differed significantly from environmental impacts. Cost analysis results are included in the SI (Table 2.6).

The scale of the treatment plant also seemed to affect operation cost. The cost per FU shows a general decrease as scale increases (Figure 2.7). This follows a similar pattern as the environmental impacts, which implies that there is a relationship between how environmental impacts and costs change with scale. Therefore, in IX systems, operation costs can potentially serve as an indicator for relative environmental impact, allowing for quick estimation of environmental impacts based on costs.

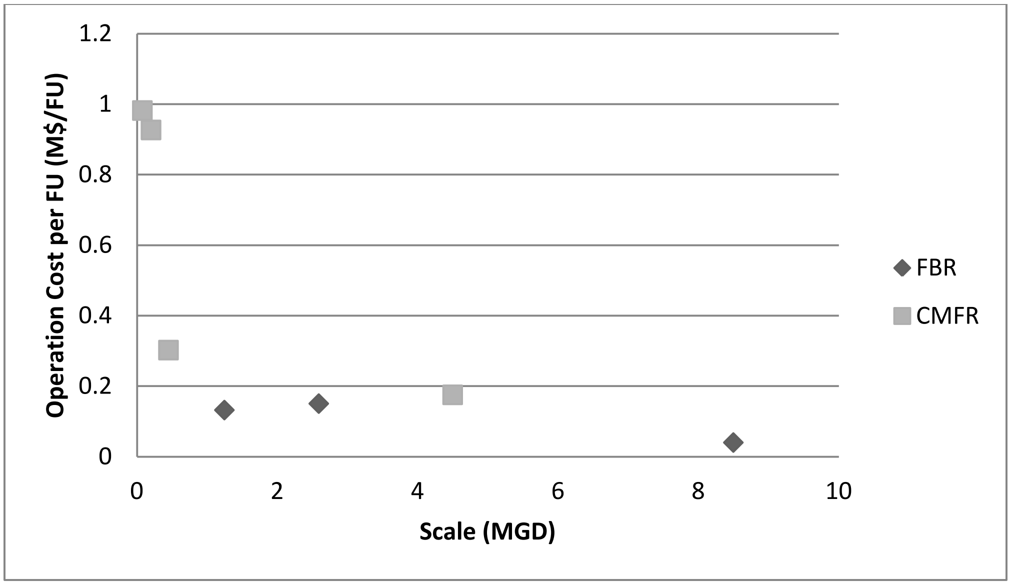

Figure 2.7: The relationship between operation cost and scale for fixed bed reactor (FBR) and completely mixed flow reactor (CMFR) ion exchange systems shows a decrease in cost as scale increases.

Although capital costs were not able to be directly collected for most of the plants, information from manufacturers as well as published technical documents indicate that capital costs of FBR systems can range from approximately $0.85 million at 2 MGD to $4.5 million at 10 MGD. CFMR systems, however, can range from approximately $ 1 million at 2 MGD to $4 million at 10 MGD (in 2015 USD) (Delphos et al., 2001; Murray et al., n.d.). Therefore, the capital costs for both systems are similar, but there is not enough data available to develop strong conclusions in this regard.

2.4 Sensitivity Analysis

To evaluate the sensitivity of assessment results to various inputs, the impacts were recalculated after individually changing each input by 10%. The relative change in the environmental impact for each impact category as well as operation cost was calculated as a percent change. The inputs tested include individual impact contributors in the life cycle inventory (i.e. electricity requirements, resins requirements, brine waste production, transport requirements, and salt requirements). Furthermore, the regeneration frequency and resin replacement rate were tested. The entire results are included in the SI (Tables 2.7-13).

The impact categories of acidification, global warming potential, and respiratory effects are most sensitive to electricity requirements, with a percent change ranging from about 2.5-8%. Salt production mainly affects eutrophication, carcinogenics, noncarcinogenics, and ecotoxicity with percent changes of 6-8%. Furthermore, brine waste treatment mainly has effects on eutrophication with percent changes over 4%. This is likely due to the release of chemicals into water bodies after being treated at the WWTP. Resin has up to 10% effect on ozone depletion in the systems, mainly due to the trichloromethane used in its production. Transport requirements mainly affect smog impacts, with up to approximately 5% change.

Changes in regeneration frequency can potentially alter assessment results, particularly for FBR systems. Therefore, a sensitivity analysis was also performed on the regeneration frequency. The highest sensitivity (8-10%) is in the categories of eutrophication, carcinogenics, noncarcinogenics, and ecotoxicity, which is expected because changes in regeneration frequency are linked closely to salt usage. A change in regeneration frequency also had a 5-8% change on operation costs.

The resin replacement rate shows changes similar to the resin requirements. Therefore, the most sensitive category is ozone depletion with 4-10% change. However, the resin replacement rate seems to affect FBR systems much more than CMFR systems, likely because the replacement rate is already high for the CMFR systems.

2.5 Conclusion

This study evaluated the environmental and economic impacts of IX systems employed in drinking water treatment plants for removal of organics, using an LCA and cost analysis approach. A life cycle inventory was developed for the operation phase of each plant as well as the construction phase of two representative plants. Impact assessment results showed that the impacts due to the operation phase of the treatment plants were significantly greater than impacts due to the construction phase over the course of 20 years or more. Therefore, the impacts of the operation phase were used to characterize the environmental impact of the treatment plants. A functional unit that takes into account both water quantity and water quality treated was used in the study. This demonstrated that the appropriate functional unit can significantly alter relative assessment results, showing a more fair comparison between the systems studied. Furthermore, it demonstrates the importance of maintaining high removal rates and, in locations where contaminant concentrations are already very low, alternative methods for contaminant removal may be preferable. The two main designs employed for IX systems are a FBR design and a CMFR design. FBR designs use less electricity, resin, and transport but require more salt and produce more brine waste, primarily because of higher regeneration requirements which can be caused by improper maintenance of resins. FBR designs therefore have higher environmental impact than CMFR systems in areas of eutrophication, carcinogenics, non-carcinogenics, and ecotoxicity. Therefore, efforts to improve sustainability of those systems are best directed toward reducing regeneration requirements. FBR systems, however, have lower operation cost than CMFR systems because of the relatively low price of salt and brine waste disposal. Environmental impacts and costs of the operation phase per FU were found to decrease as scale increases, likely due to higher efficiency of pumping and mixing at larger scales. Furthermore, because they follow similar trends with scale, operation costs can be used to make a relative estimate of environmental impact.

Similar conclusions can likely extend to IX systems that remove other types of contaminants. For example, in most IX systems it is likely that the environmental impacts of the operation phase is dominant over the construction phase, both operation cost and environmental impact decrease with scale, and using a functional unit that takes into account both water quality and quantity will be appropriate. Conclusions related to the comparison between FBR and CMFR designs, however, may not be generalized when there is no regeneration performed, such as when using selective IX for perchlorate removal.

2.6 References

Ali, I., Gupta, V. K., 2007. Advances in Water Treatment by Adsorption Technology. Nature Protocols. 1, 2661-2667.

Bare, J. C., Norris, G. A., Pennington, D. W., McKone, T., 2003. TRACI – The Tool for the Reduction and Assessment of Chemical and other Environmental Impacts. Journal of Industrial Ecology. 6, 49-78.

Bare, J., Gloria, T., Norris, G., 2006. Development of the Method and U.S. Normalization Database for Life Cycle Impact Assessment and Sustainability Metrics. Environmental Science and Technology. 40, 5108-5115.

Barrios, R., Siebel, M., Helm, A., Bosklopper, K., Gijzen, H., 2008. Environmental and financial life cycle impact assessment of drinking water production at Waternet. Journal of Cleaner Production, 16, 471-476.

Canedo-Arguelles, M., Kefford, B.J., Piscart, C., Prat, N., Schafer, R.B., Schulz, C.J., 2013. Salinisation of rivers: An urgent ecological issue. Environmental Pollution. 173, 157-167.

Choe, J. K., Mehnert, M., Guest, J., Strathmann, T. J., Werth, C. J., 2013. Comparative Assessment of the Environmental Sustainability of Existing and Emerging Perchlorate Treatment Technologies for Drinking Water. Environmental Science and Technology. 47, 4644-4652.

Clifford, D., Liu, X., 1993. Ion Exchange for Nitrate Removal. Journal of American Water Works Association. 85, 135-143.

Clifford, D., Sorg, T.J., Ghurye, G.L., 2011. Ion exchange and adsorption of inorganic contaminants, in: Edzwald, J.K. (Ed.), Water quality & treatment: A handbook on drinking water, sixth ed. New York, NY.

Curran, M., 2012. Life Cycle Assessment Handbook: A guide for environmentally sustainable products. Beverly, Mass.: Scrivener Publishing.

Diaz, N., Helu, M., Jarvis, A, Tönissen, S., Dornfeld, D., Schlosser, R., 2009. Strategies for Minimum Energy Operation for Precision Machining.*Laboratory for Manufacturing and Sustainability*. UC Berkeley: Laboratory for Manufacturing and Sustainability.

Delphos, P., Harr, K., Bianco, T.L., 2001. Selective DBP Precursor Removal with an Innovative Ion Exchange Process. American Water Works Association.

Dominguez-Ramos, A., Chavan, K., García, V., Jimeno, G., Albo, J., Marathe, K. V., Yadav, G. D., Irabien, A., 2014. Arsenic Removal from Natural Waters by Adsorption or Ion Exchange: An Environmental Sustainability Assessment. Industrial and Engineering Chemistry Research 53, 18920-18927.

EERC (version 2.0-13). Applied Economics Office, National Institute of Standards and Technology. Available from http://energy.gov/eere/femp/eerc-download

European Environment Agency, 2012. Towards Efficient Use of Water Resources in Europe. Copenhagen.

Ghurye, G.L., Clifford, D.A., Tripp, A.R., 1999. Combined Arsenic and Nitrate Removal by Ion Exchange. Journal of American Water Works Association. 91, 85-96.

Gu, B.H., Ku, Y.K., Brown, G.M., 2005. Sorption and Desorption of Perchlorate and U(vi) by Strong-Base Anion-Exchange Resins. Environmental Science and Technology. 39, 901-907

Hsu, S., Singer, P.C., 2010. Removal of Bromide and Natural Organic Matter by Anion Exchange. Water Research. 44, 2133-2140.

ISO., 2006a. Environmental management—Life cycle assessment: Principles and framework. ISO14040. Geneva: International Standard Organisation.

ISO., 2006b. Environmental management—Life cycle assessment: Requirements and Guidelines. ISO14044. Geneva: International Standard Organisation.

Lundin, M., Bengtsson, M., Molander, S., 2000. Life Cycle Assessment of Wastewater Systems: Influence of System Boundaries and Scale on Calculated Environmental Loads. Environmental Science and Technology. 34, 180-186.

Maul, G., Kim, Y., Amini, A., Zhang, Q., Boyer, T., 2014. Efficiency and Life Cycle Environmental Impacts of Ion-exchange Regeneration Using Sodium, Potassium, Chloride, and Bicarbonate Salts. Chemical Engineering Journal. 254, 198-209.

Murray, B., Pieterse, S., Raymer, D., Swartz, C., n.d. An Evaluation of MIEX Resin Technology for Potable Treatment of Highly Coloured Raw Waters throughout the Cap Region of South Africa. Orica Advanced Water Technologies Pty.

Panswad, T., Anan, C., 1999. Impact of High Chloride Wastewater on an Anaerobic/anoxic/aerobic process with and without Inoculation of Chloride Acclimated Seeds. Water Research. 33, 1165-1172.

Ras, C., von Blottnitz, H., 2012. A comparative life cycle assessment of process water treatment technologies at the Secunda industrial complex, South Africa. Water SA. 38, 549-554.

Rengaraj, S., Moon, S.H., 2002. Kinetics of Adsorption of Co(ii) Removal from Water and Wastewater by Ion Exchange Resins. Water Research. 36, 1783-1793.

United Nations Environment Programme and International Water Management Institute. (2011). Ecosystems for Water and Food Security. Nairobi and Colombo.

United States Environmental Protection Agency (USEPA)., 2012. 2012 National Public Water Systems Compliance Report (EPA DOCUMENT 305R14001).Washington, DC: Office of Enforcement and Compliance Assurance (2201A).

Urbansky, E. T., 2002. Perchlorate as an environmental contaminant. Environmental Science and Pollution Research. 9, 187-192.

Vince, F., Aoustin, E., Bréant, P., Marechal, F., 2008. LCA tool for the environmental evaluation of potable water production. Desalination. 37-56.

2.7 Supplementary Information

Assumptions were made in this study where detailed data or information were not available and the effect of the assumption was not likely to affect the conclusions.

Table 2.2: Assumptions made in the life cycle inventory and their justifications

Assumption	Justification
Both conventional and MIEX resins are disposed of by incineration.	This is the standard method of resin disposal. Life cycle inventories were available in Ecoinvent 3. Even if resin was sent to solid waste management, many municipalities incinerate solid waste.
Both conventional and MIEX resin have the same environmental impact and can be approximated by a generic polystyrene resin	The main difference between them is the material (polysterene and polyacrylcic) and iron oxide. Ecoinvent 3 inventories are available for polystyrene resin. Comparison between new material inventories created using polyacrylic showed negligible differences.
The lifetime chosen was 20 years	This is the lifetime of the CMFR plants (the lifetime of the FBR plants is 30 years)
Electricity costs are $0.09 per kWh	Commercial and Industrial Electricity Costs in Florida range from $0.08-0.10 per kWh
The FBR plants perform a caustic clean every 3 years	This was prescribed in the systems manuals
Transport land distance of 150 km by Truck used to estimate distance from a port to the treatment plant.	Salt and resin are transported to ports by ship (e.g. Port Canaveral) before being transported to the facility by truck. Distance of most of the plants from ports ranges from 50-200 km.

Table 2.3: Construction phase life cycle inventory for plant A

Item	Amount	Units	Material
Vessels	87500	lbs	Steel, low-alloyed, at plant/RER S
Bleed Tank	1330.5	lbs	Polyethylene, HDPE, granulate, at plant/RER S
Control panel	802.3	lbs	Electronics
Brine Pumps	2	pieces	
Brine Storage Tank	1330.5	lbs	Polyethylene, HDPE, granulate, at plant/RER S
Brine supply valves	55.2	g	Polyvinylchloride, bulk polymerised, at plant/RER S
Brine system booster pump	2033.62	USD	Pumps and compressors
caustic dilution mixer	5	lbs	Polyvinylchloride resin (B-PVC), bulk polymerisation, production mix, at plant RER
Caustic pump	1190	USD	Pumps and compressors
Clean in place tank (caustic makeup)	104	lbs	Polyethylene, HDPE, granulate, at plant/RER S
Valves	1327	kg	Cast iron, at plant/RER S
Salt Silo	25	ton	Glass fibre reinforced plastic, polyamide, injection moulding, at plant/RER S
Transfer pumps	202063	USD	

Table 2.4: Construction phase life cycle inventory for plant G

Item	Amount	Units	Material
Air actuated valves	66.72	lb	Polyvinylidenchloride, granulate, at plant/RER U
Contactor Vessel Agitator	545	lb	Steel, low-alloyed, at plant/RER S
Control panel	802.3	lb	Electronics
IX vessel	1000	lb	Glass fibre reinforced plastic, polyamide, injection moulding, at plant/RER U
Pumps	4	pieces	
Regeneration Tank	616.0266	lb	Glass fibre reinforced plastic, polyamide, injection moulding, at plant/RER U
Regeneration Vessel Agitator	138	lb	Steel, low-alloyed, at plant/RER S
Resin Transfer Tank	200	lb	Polyethylene, HDPE, granulate, at plant/RER U
Salt Saturator Tank	271.51	lb	Polyethylene, HDPE, granulate, at plant/RER U

Table 2.5: Life cycle inventory (for operation phase)

	A	B	C	D	E	F	G	H
Total Electricity (kWh/20yrs)	12,182,887	4,002,862	2,927,387	2,629,471	735,115	437,388	622,568	258,662
Total Salt (tons/20yrs)	14,832	15,830	9,967	7,200	1,440	719	302	48
Total Brine Waste (gallons/20yrs)	73,992,711	83,634,612	134,339,212	32,850,000	3,438,300	988,653	607,068	277,400
Resin addition (kg/20yrs)	62,323.89	26,710.24	26,710.24	298,689.97	42,088.44	50,929.21	15,187.19	12,198
Transport (tkm/ 20yrs)	30,665,757	32,088,940	20,362,618	20,045,240	3,785,569	2,400,603	891,837	326,549
NaOH (kg/20yrs)	31,852	13,651	13,651	-	-	-	-	-
HCl (kg/20yrs)	-	-	-	-	9,948	-	-	-

Table 2.6: Lifetime operation cost results

	A	B	C	D	E	F	G	H
Lifetime Operation Cost	$ 2,226,075	$ 1,616,792	$ 1,107,996	$ 2,326,855	$ 596,458	$398,773	$ 250,056	$ 118,659

Table 2.7: Sensitivity analysis for 10% change in regeneration frequency

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	0.26%	0.62%	0.42%	0.03%	0.04%	0.02%	0.02%	0.00%
Global warming	3.87%	6.80%	6.60%	5.75%	6.72%	4.62%	4.69%	2.26%
Smog	5.83%	8.21%	8.05%	6.88%	7.55%	5.72%	5.49%	2.68%
Acidification	2.20%	5.04%	4.91%	5.95%	6.97%	4.97%	4.61%	2.44%
Eutrophication	9.53%	9.84%	9.85%	8.55%	8.80%	7.42%	7.86%	4.91%
Carcinogenics	8.96%	9.64%	9.62%	8.27%	8.65%	7.28%	7.42%	4.16%
Non carcinogenics	8.90%	9.62%	9.62%	8.63%	8.91%	7.75%	7.67%	4.65%
Respiratory effects	4.51%	7.34%	7.21%	7.03%	7.69%	5.94%	5.29%	2.76%
Ecotoxicity	9.41%	9.80%	9.76%	8.64%	8.97%	7.85%	8.07%	4.87%
Fossil fuel depletion	5.14%	7.75%	7.52%	5.65%	6.57%	4.45%	4.76%	2.12%
Operation Cost	4.77%	7.17%	6.63%	2.58%	3.59%	2.60%	2.18%	0.82%

Table 2.8: Sensitivity analysis for 10% change in resin replacement rate

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	10.82%	10.42%	10.65%	9.97%	7.06%	4.27%	8.78%	4.24%
Global warming	0.26%	0.18%	0.26%	2.71%	1.31%	1.44%	1.24%	1.14%
Smog	0.21%	0.11%	0.17%	2.16%	1.06%	1.25%	1.25%	1.25%
Acidification	0.09%	0.07%	0.11%	1.30%	0.56%	0.67%	0.42%	0.40%
Eutrophication	0.17%	0.07%	0.08%	1.38%	0.79%	1.05%	1.51%	1.85%
Carcinogenics	0.18%	0.08%	0.11%	1.54%	0.82%	1.03%	1.42%	1.76%
Non carcinogenics	0.13%	0.06%	0.07%	1.14%	0.61%	0.80%	1.05%	1.38%
Respiratory effects	0.13%	0.08%	0.12%	1.39%	0.66%	0.80%	0.64%	0.65%
Ecotoxicity	0.15%	0.06%	0.09%	1.26%	0.66%	0.85%	1.23%	1.73%
Fossil fuel depletion	0.39%	0.23%	0.34%	3.36%	1.71%	1.82%	1.91%	1.70%
Operation Cost	1.82%	1.08%	1.57%	7.04%	3.98%	3.00%	4.25%	3.47%

Table 2.9: Sensitivity analysis for 10% change in electricity requirements

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Global warming	5.63%	2.91%	3.12%	2.76%	3.73%	3.36%	6.67%	6.58%
Smog	3.80%	1.61%	1.77%	1.72%	2.38%	2.28%	5.29%	5.68%
Acidification	7.38%	4.69%	4.93%	4.91%	5.93%	5.80%	8.39%	8.60%
Eutrophication	0.30%	0.10%	0.08%	0.12%	0.20%	0.21%	0.72%	0.94%
Carcinogenics	0.83%	0.27%	0.28%	0.34%	0.50%	0.52%	1.64%	2.19%
Non carcinogenics	0.94%	0.31%	0.30%	0.40%	0.59%	0.63%	1.93%	2.72%
Respiratory effects	5.14%	2.48%	2.65%	2.80%	3.68%	3.67%	6.81%	7.42%
Ecotoxicity	0.44%	0.14%	0.15%	0.18%	0.26%	0.27%	0.91%	1.37%
Fossil fuel depletion	4.31%	1.95%	2.13%	1.75%	2.50%	2.16%	5.26%	5.04%
Operation Cost	4.92%	7.23%	6.64%	2.28%	3.13%	2.34%	1.57%	0.53%

Table 2.10: Sensitivity analysis for 10% change in salt requirements

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	0.25%	0.60%	0.38%	0.03%	0.04%	0.02%	0.02%	0.00%
Global warming	2.45%	4.10%	3.79%	2.70%	2.61%	1.97%	1.16%	0.44%
Smog	2.60%	3.58%	3.38%	2.65%	2.62%	2.10%	1.44%	0.59%
Acidification	1.63%	3.37%	3.05%	2.44%	2.11%	1.73%	0.74%	0.29%
Eutrophication	6.78%	6.89%	4.84%	6.18%	7.13%	6.43%	6.37%	3.20%
Carcinogenics	7.56%	8.07%	7.11%	6.87%	7.30%	6.31%	5.95%	3.03%
Non carcinogenics	7.21%	7.72%	6.53%	6.88%	7.30%	6.57%	5.93%	3.19%
Respiratory effects	4.29%	6.72%	6.19%	5.26%	4.95%	4.13%	2.27%	0.94%
Ecotoxicity	8.46%	8.78%	8.30%	7.70%	8.02%	7.11%	7.04%	4.06%
Fossil fuel depletion	2.33%	3.42%	3.23%	2.14%	2.18%	1.58%	1.13%	0.42%
Operation Cost	4.92%	7.23%	6.64%	2.28%	3.13%	2.34%	1.57%	0.53%

Table 2.11: Sensitivity analysis for 10% change in brine waste production

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	0.01%	0.02%	0.03%	0.00%	0.00%	0.00%	0.00%	0.00%
Global warming	0.10%	0.17%	0.40%	0.10%	0.05%	0.02%	0.02%	0.02%
Smog	0.11%	0.16%	0.38%	0.10%	0.05%	0.02%	0.02%	0.03%
Acidification	0.07%	0.15%	0.35%	0.10%	0.04%	0.02%	0.01%	0.01%
Eutrophication	2.50%	2.69%	4.82%	2.08%	1.26%	0.65%	0.94%	1.37%
Carcinogenics	0.72%	0.82%	1.84%	0.60%	0.33%	0.17%	0.23%	0.34%
Non carcinogenics	0.99%	1.12%	2.42%	0.86%	0.48%	0.25%	0.33%	0.51%
Respiratory effects	0.16%	0.27%	0.62%	0.18%	0.09%	0.04%	0.03%	0.04%
Ecotoxicity	0.31%	0.34%	0.81%	0.25%	0.14%	0.07%	0.10%	0.17%
Fossil fuel depletion	0.07%	0.11%	0.26%	0.06%	0.03%	0.01%	0.01%	0.01%
Operation Cost	Cost of brine disposal was negligible for most systems							

Table 2.12: Sensitivity analysis for 10% change in resin requirements

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	9.74%	9.38%	9.58%	9.97%	9.96%	9.98%	9.98%	10.00%
Global warming	0.19%	0.13%	0.18%	2.03%	1.38%	2.53%	1.05%	2.01%
Smog	0.08%	0.05%	0.07%	0.84%	0.58%	1.14%	0.55%	1.15%
Acidification	0.05%	0.05%	0.07%	0.81%	0.49%	0.98%	0.30%	0.59%
Eutrophication	0.14%	0.06%	0.06%	1.28%	1.04%	2.28%	1.60%	4.07%
Carcinogenics	0.14%	0.06%	0.09%	1.29%	0.96%	2.02%	1.35%	3.47%
Non carcinogenics	0.09%	0.04%	0.05%	0.87%	0.65%	1.41%	0.91%	2.46%
Respiratory effects	0.10%	0.07%	0.10%	1.25%	0.83%	1.68%	0.65%	1.38%
Ecotoxicity	0.11%	0.05%	0.07%	1.02%	0.75%	1.62%	1.13%	3.31%
Fossil fuel depletion	0.26%	0.15%	0.23%	2.31%	1.66%	2.92%	1.49%	2.75%
Operation Cost	1.64%	0.97%	1.41%	7.04%	5.61%	7.01%	4.83%	8.18%

Table 2.13: Sensitivity analysis for 10% change in transport requirements

Impact category	A	B	C	D	E	F	G	H
Ozone depletion	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Global warming	1.63%	2.69%	2.50%	2.42%	2.21%	2.12%	1.10%	0.96%
Smog	3.41%	4.60%	4.39%	4.68%	4.36%	4.46%	2.70%	2.55%
Acidification	0.86%	1.74%	1.59%	1.74%	1.42%	1.47%	0.56%	0.50%
Eutrophication	0.27%	0.27%	0.19%	0.34%	0.37%	0.42%	0.37%	0.42%
Carcinogenics	0.74%	0.77%	0.68%	0.90%	0.90%	0.99%	0.83%	0.97%
Non carcinogenics	0.77%	0.81%	0.69%	0.99%	0.99%	1.13%	0.90%	1.12%
Respiratory effects	0.31%	0.47%	0.44%	0.51%	0.45%	0.48%	0.23%	0.22%
Ecotoxicity	0.69%	0.70%	0.67%	0.84%	0.83%	0.93%	0.81%	1.08%
Fossil fuel depletion	3.03%	4.37%	4.15%	3.74%	3.60%	3.32%	2.11%	1.78%
Operation Cost	No cost change because transport costs are included in material costs							

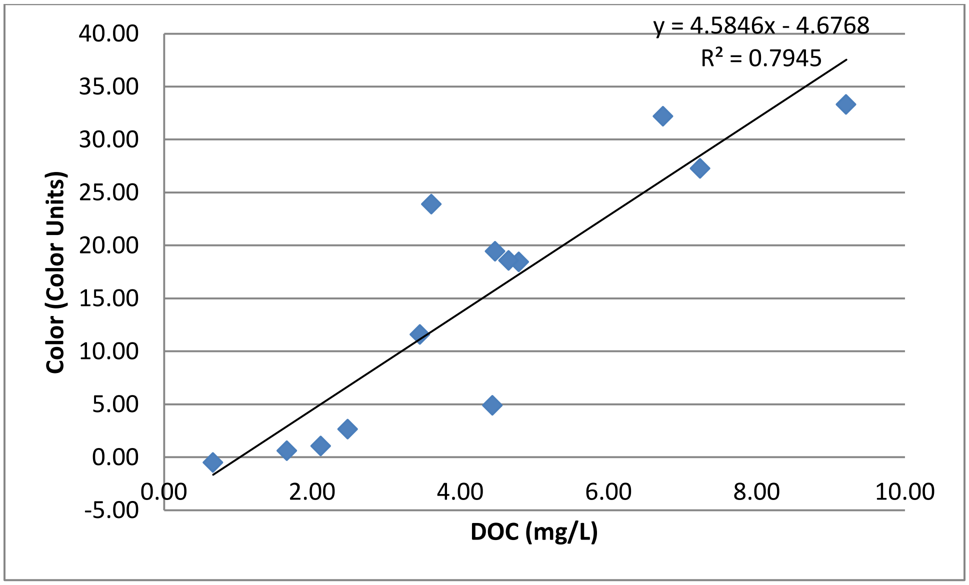

Figure 2.8: Regression plot of color vs DOC for Florida groundwater samples

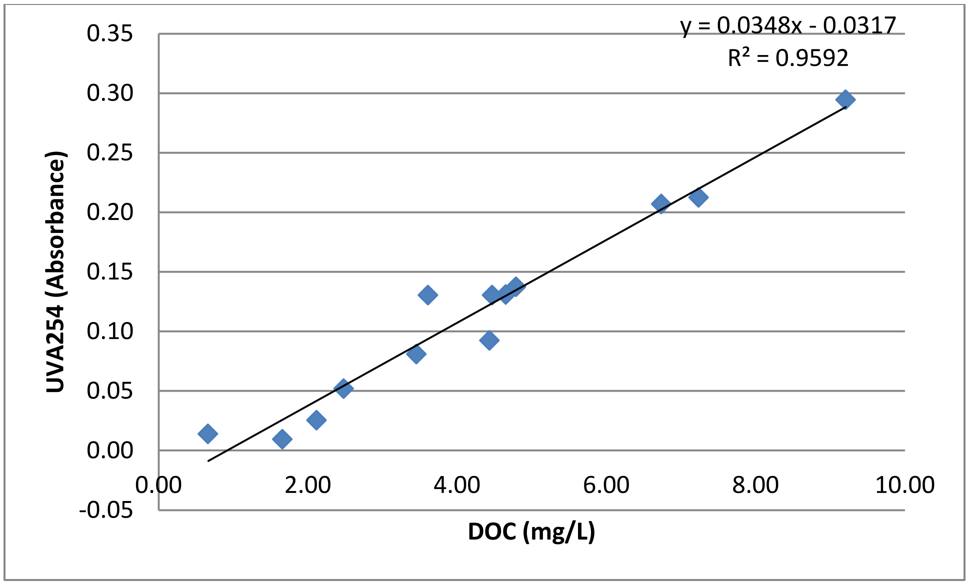

Figure 2.9: Regression plot of UVA254 vs DOC for Florida groundwater samples

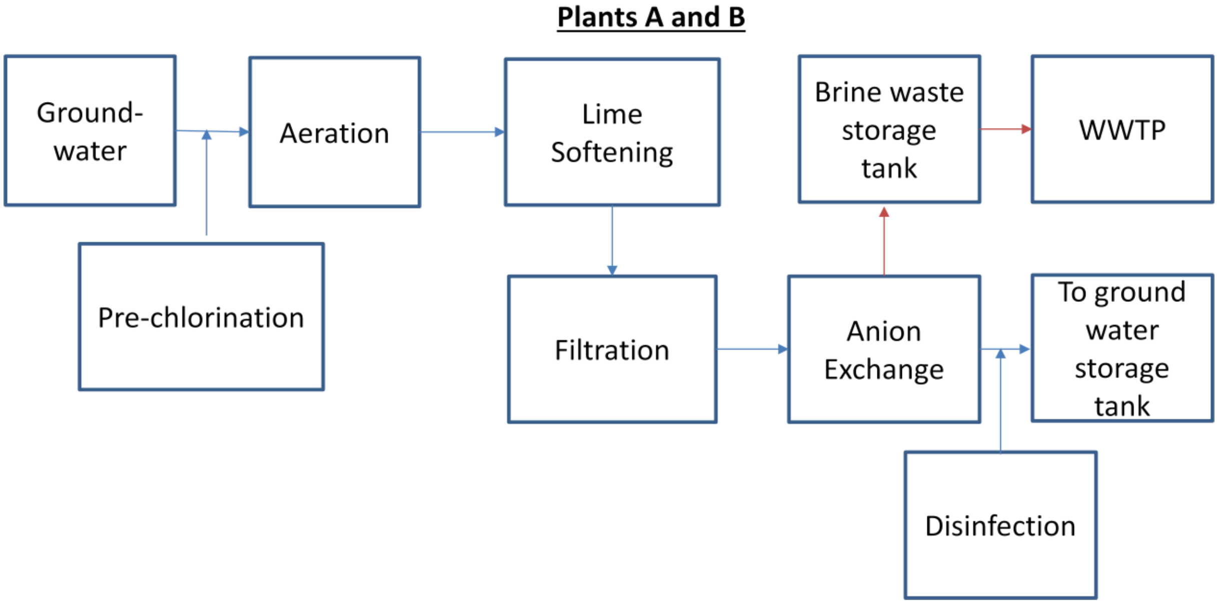

Figure 2.10: Flow diagram for plants A and B

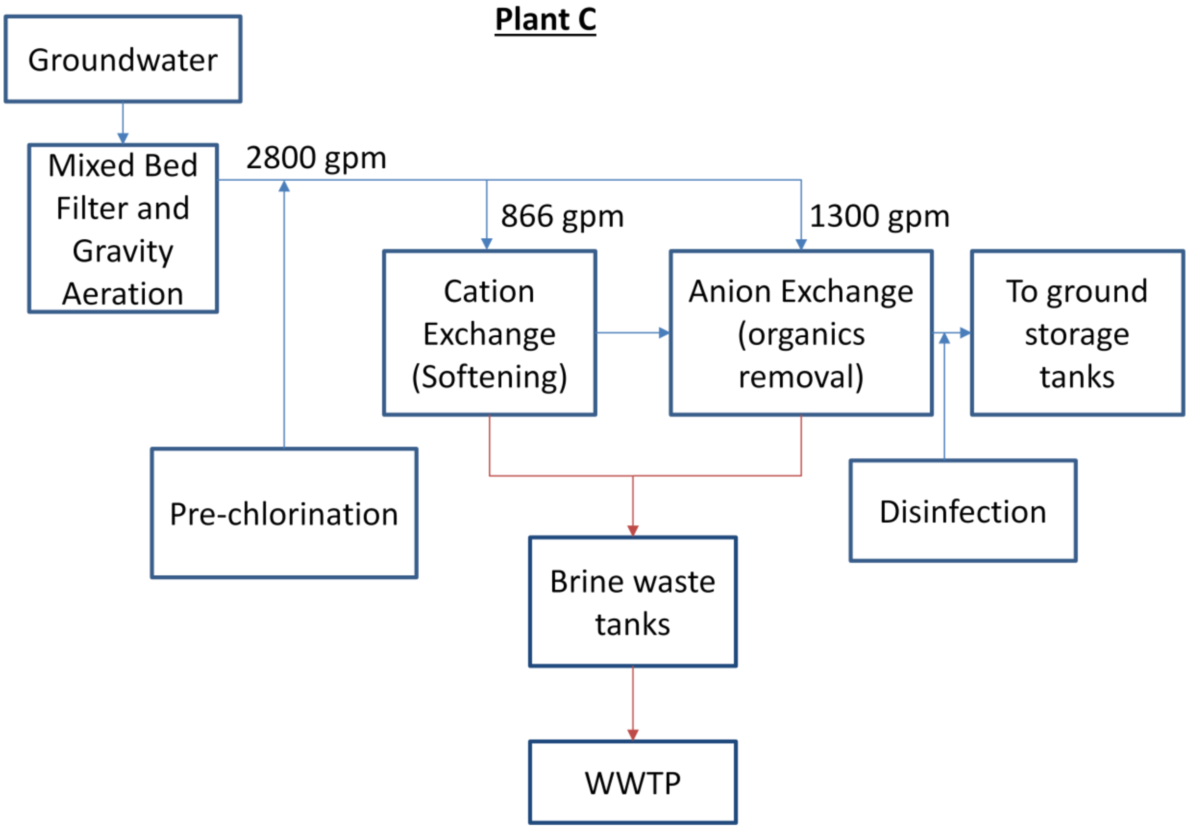

Figure 2.11: Flow diagram for plant C

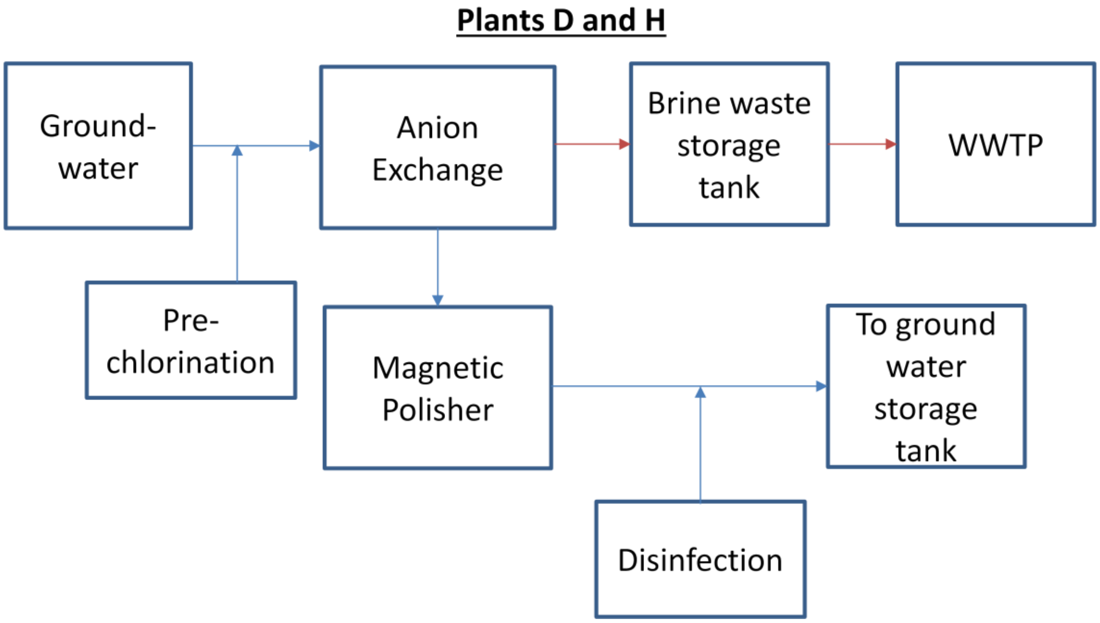

Figure 2.12: Flow diagram for plants D and H

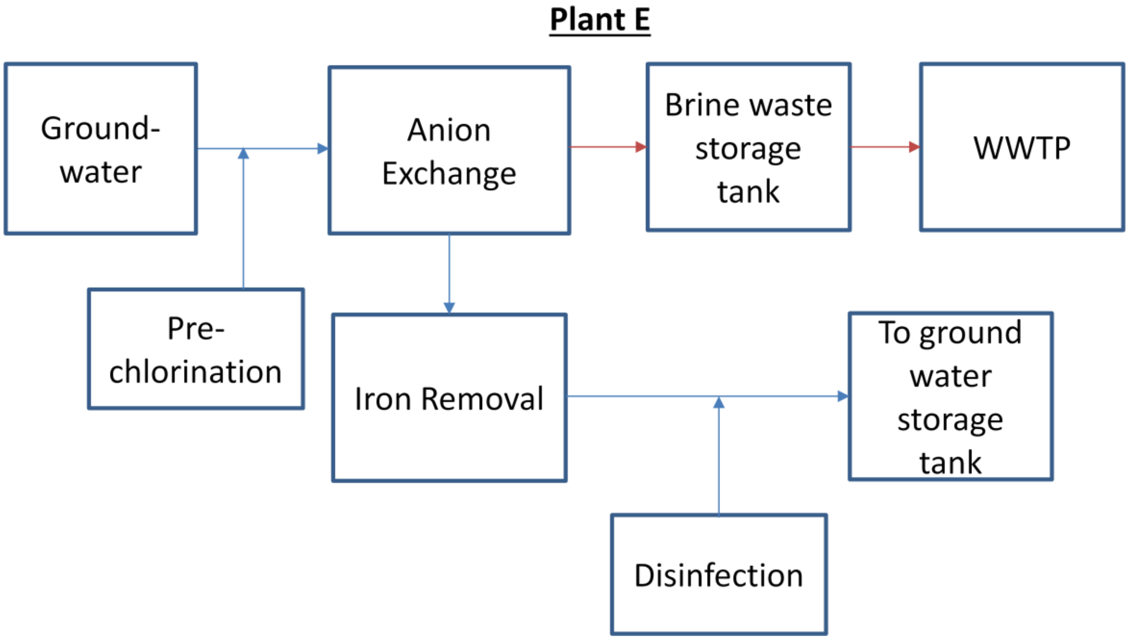

Figure 2.13: Flow diagram for plant E

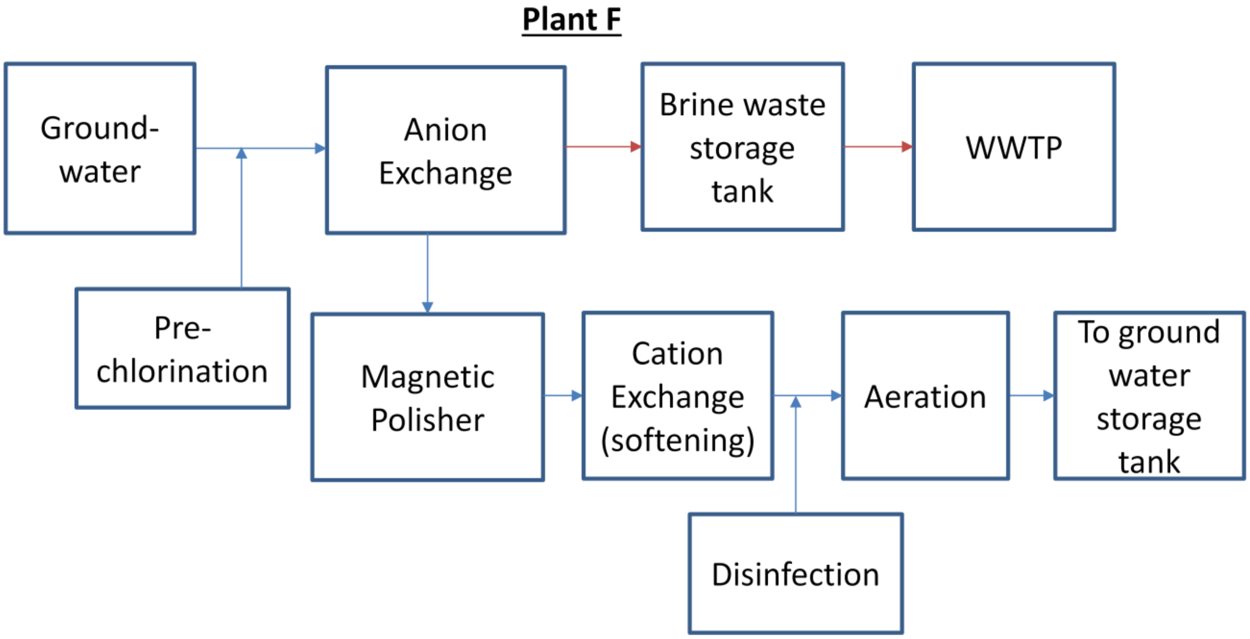

Figure 2.14: Flow diagram for plant F

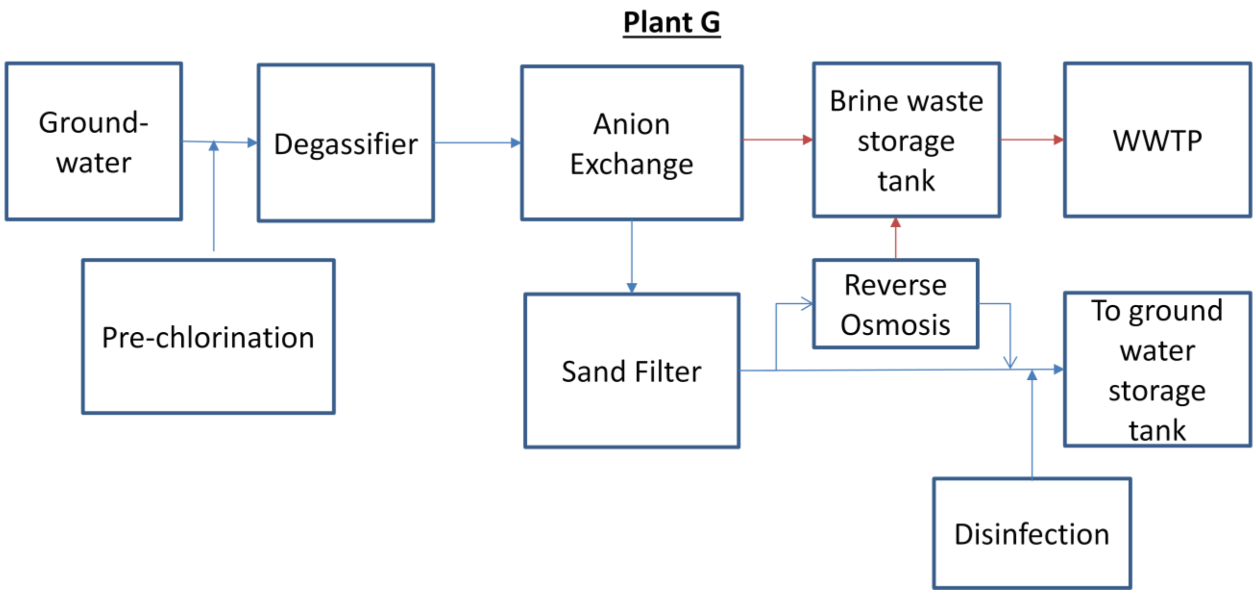

Figure 2.15: Flow diagram for plant G

Chapter 3: Integration of Process Models with Life Cycle Environmental Impact and Cost Assessment for Improving Design of Water Treatment Technology (Task 2)

3.1 Introduction

Human population growth and economic development are increasing water demands across the globe while causing water resources to become increasingly scarce (Vorosmarty et al., 2000). This places increased responsibility on potable water systems to provide environmentally and economically sustainable water treatment. Micro-economic and technical considerations have traditionally been paramount in the design of water treatment systems. Furthermore, environmental and economic evaluations have been performed on existing designs of water treatment technology. However, improved methods are needed that allow environmental and economic considerations to contribute directly to possible design improvement, rather than post-design evaluations.

Ion exchange (IX) technology serves as an example of this. IX is a type of water treatment technology that has a number of technical advantages due to adaptability for removal of various contaminants and flexibility of design, size, and implementation. Previous studies have investigated the environmental impacts and costs of current IX systems (Amini et al., 2015; Choe et al., 2013; Ras and von Blottnitz, 2012; Dominguez-Ramos et al., 2014) using life cycle assessment (LCA), a tool that allows for quantification of environmental burdens. Some of the main benefits of using LCA are related to its ability to avoid unintended shifting of burdens or impacts from one area of the life cycle to another. LCA, therefore, avoids the issues of only taking into account site-specific considerations (e.g. only emissions at a particular plant instead of due to the materials and process upstream) (Azapagic et al., 1999). However, in order to improve IX design based on the understanding that LCA can provide, improved methods are needed that can allow LCA to play a part in identifying design trends that are more sustainable.

Azapagic et al. (2006) have outlined the importance of systematically integrating LCA into process design rather than considering it as an ‘add on’, and have proposed the use of LCA in optimization methods. It was also conceptualized that both LCA and economic conditions should be taken into account together; however, this has been lacking in current research (Fazeni et al., 2014). Furthermore, Life Cycle Costing Analysis (LCCA), which takes into account expenses over the entire life of the system in particular is lacking and should be incorporated into evaluation and design (Fazeni et al., 2014). Therefore, improved methods are needed to take into account both LCA and LCCA in design improvement.

The optimization of products and processes requires a variety of alternative choices as well as criteria and constraints. Process modeling is a method that allows for evaluation of potential scenarios due its dynamic ability to project the effects of a wide range of design changes. Although process modeling results have been tied to environmental indicators by previous researchers (Vince et al., 2008), there has never been a tight integration of process modeling with LCA as well as LCCA. This would allow for direct estimation or environmental impacts and costs based on design choices, instead of by proxy indicators. Furthermore, it would allow for avoidance of the shifting of burdens and impacts across the life cycle.

The purpose of this study is to develop a model that integrates process modeling with LCA and LCCA to allow for evaluation of trends in design choices that can improve environmental and economic sustainability. This can help to identify the most important design parameters for improving the system. The model will be applied to IX water treatment systems;

however, the general modeling framework can also be applied to other types of water treatment technology. This also expands the knowledge base on the sustainability of IX technology, for which there are few previous studies (Amini et al., 2015). Providing a link between an integrated process model and environmental impact and cost assessment also provides a valuable tool for both academics and practitioners to use in identifying and selecting improved IX designs. Although initially the model will be developed based on IX systems that remove organics, the academic community will be able to add complexity to the code, such as IX systems that remove other types of contaminants, as further studies on the sustainability of other IX applications are carried out. Furthermore, this model can provide the foundation for a user-friendly tool that drinking water professionals can potentially use in practice.

3.2 Methodology

3.2.1 Model Description

This research dynamically links process models with LCA and LCCA to allow for estimation of environmental impacts and costs of IX drinking water technology that uses various design parameters. Therefore, the environmental impacts and costs for a particular design scenario can be estimated in a streamlined method without the time consuming and difficult process of performing an LCA and LCCA for each scenario individually. In addition, the model allows for optimal design choices or trends to be identified, leading to overall improvement of the sustainability of IX design.

The current integrated model allows for the estimation of environmental impacts and costs of IX systems for removal of organics in order to prevent disinfection byproducts. Two main reactor types are considered, which are commonly used with these systems: a fixed bed reactor (FBR) and a completely mixed flow reactor (CMFR). However, the model is modular and can be expanded by future researchers to include other reactor configurations as well as IX systems that remove other types of contaminants. While this research applies the linking of process models with LCA and LCCA for IX systems, the method can also be applied to wide variety of water treatment technology to identify design options that improve environmental and economic sustainability.

The process models used in the integrated model have been developed by Zhang et al. (2015) and Hu & Boyer (2017). The models consider transport mechanisms (e.g., advection, dispersion) and external mass transport at the macroscale for liquid phase and diffusive mass transfer for resin particles (solid phase) at the microscale. The model developed by Zhang et al. (2015) is primarily for FBR configurations while model developed by Hu & Boyer (2017) is primarily for CMFR systems.

The information for the LCA and LCCA is from life cycle inventories (LCIs) developed for IX water treatment plants for organics removal in Florida, described in Amini et al. (2015). These inventories include data from eight treatment plants that range in scale from 0.078 million gallons per day (MGD) capacity to 8.5 MGD average flow and utilized both FBR and CMFR configurations. A wealth of data was provided from these plants that allowed for development of the model that can account for variations in flow rates, reactor configurations, operation and maintenance, and so on.

3.2.1.1 Model Inputs

The model inputs include a number of design parameters that can be modified to evaluate a particular design scenario. These decision variables are the alternative design choices for the system and through consultation with drinking water treatment plant superintendents and operators that use IX, as well as engineering firms that design IX systems. The decision variables, the reactor type that they primarily apply to, and an example of possible values are shown in Table 3.1. Each of the decision variables generally applies to one of the reactor types or both, because the design of each reactor configuration differs significantly. Two types of regenerant are considered, which can be used for both types of reactors. NaCl is the conventional regenerant choice while $NaHCO_3$ is a potential alternative. The two options vary significantly in cost as well as environmental impact. The LCI information for the regenerant are found in Maul et al. (2014). The hydraulic retention time (HRT) is a design characteristic of both types of reactors and can affect effectiveness of treatment as well as reactor size. Resin radius is also taken into account for both options and can affect effectiveness of treatment. Generally, resin attrition will increase as smaller resin sizes are used; however, this is not currently taken into acount in the model. However, an estimated resin attrition rate can be entered for FBR systems. Such attrition is not an intended design criteria but can significantly affect operation of FBR systems over time. This is not, however, applied to CMFR systems because these systems are designed with expected attrition, typically 2 gallons of resin per 1 MG of water treated. Resin cleaning frequency is also taken into account for FBR systems. Amini et al. (2015) found this to be an important variable that contributes to the regeneration rate of FBR systems which highly influences environmental impacts and costs, but was not particularly relevant to CMFR systems because the resin is continually replaced. Regeneration ratio, resin volume convention in IX reactor, and resin volume concentration in regeneration reactor are considered specifically in CMFR systems. These can affect treatment effectiveness as well as reactor size. It should be noted that a number of other design criteria could be taken into account when evaluating IX systems; however, through consultation with water professionals and engineers, these were considered to be of most interest. The model, however, can be modified to include other decision variables as well. The model input file is designed simply to allow for selection of the decision variables.

3.2.1.2 Model Structure

The model may be divided into three primary sections, which are shown in Figure 3.1. The first section defines standard values and converts the given inputs to the model into a format that can be utilized by the model. This may involve conversion of units, changes in format, and so on. The second section runs the process model and LCA/LCCA. The second section of the model can further be divided into six sub-sections which include the process model calculation, the LCA, and the LCCA for both FBR and CMFR systems. Furthermore, each of these subsections has their respective steps. For example, the LCA subsection also includes calculation of the LCI results for the particular scenario as well as the environmental impact assessment step. The third section of the model compiles outputs from the model and generates an output file with the results.

3.2.2 Model Utilization

The model can currently be run using one of three methods. The first is the calculation of a single design scenario using one input file. This is the most simple use of the model and can estimate the environmental impacts and costs of a single scenario. The second method involves running the total number of permutations of decision variable options, given a range of options for each input. This method is used to allow for analysis of trends in the results and develop conclusions regarding the relationship between the various design choices. The third method involves the use of an optimization method to select an optimal design, given a range of input options, without having to run all of the possible permutations. The latter two methods are described in the following sections.

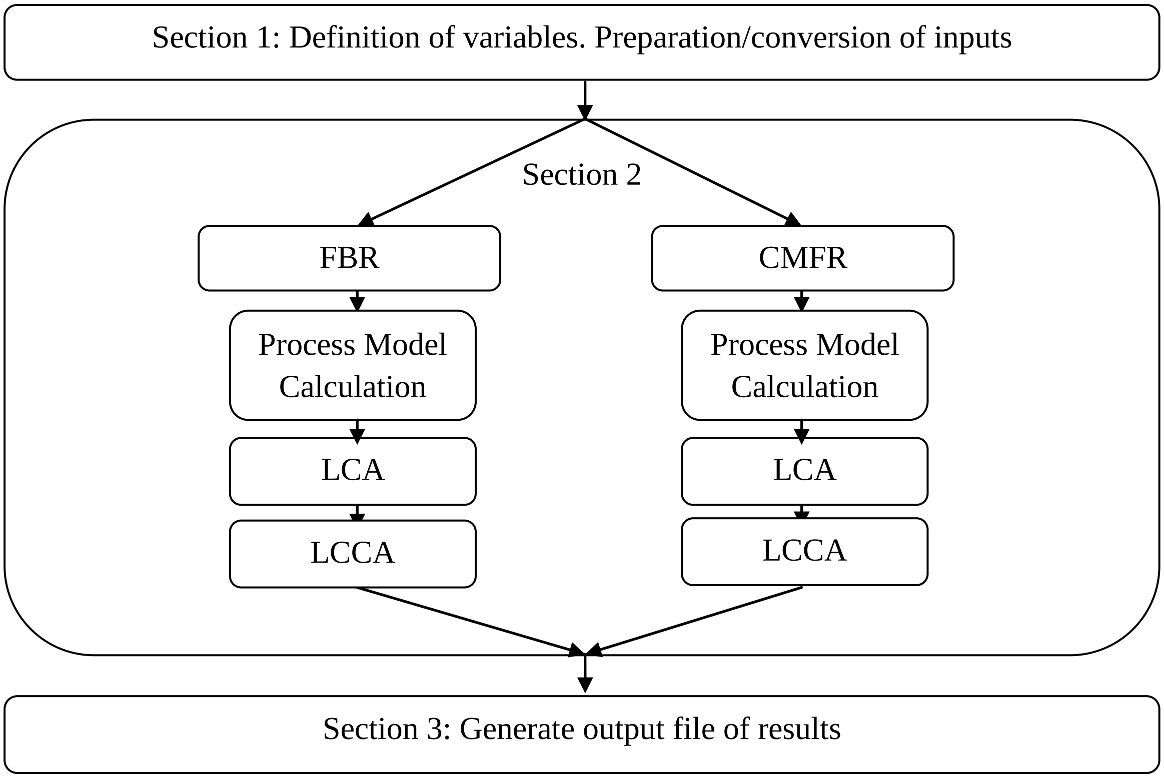

Figure 3.1: Model structure

3.2.2.1 Multiple Permutation Analysis

This method of model utilization allows for running a large number of input permutations. This requires selecting a range of input options. For example, a range of choices for HRT can be selected. For this research, discrete options were used to minimize the number of permutations. Therefore, a given input may have five potential options selected instead of a full range of options. This decreases significantly the number of computations required, the time for computation, and the amount of data generated. However, it still provides an understanding of key choices for the inputs and how they relate to the environmental impacts and costs of the system. The decision variables with the options that were selected for the purpose of this research are shown in Table 3.1.

The number of input options leads to 12,000 possible permutations of design scenarios. In order to calculate each of these scenarios a separate code was developed to generate a unique input file for each of the possible permutations. After the input files were generated, they were each run and the results were compiled in an output file. To account for the large number of files and long computation time, these codes were run using University of South Florida's research computing cluster. The permutations were submitted in a parallel manner to reduce computation time. The time for computation of each design scenario varied but was typically less than 10 minutes in duration.

Table 3.1: Decision variables and input options of the model developed in task 2

Decision variable	**Reactor type it applies to**	**Selected Options**	**Units**
Reactor Type	-	FBR, CMFR	-
Regenerant Type	FBR, CMFR	NaCl, NaHCO3-	-
Hydraulic Retention Time of the Reactor	FBR, CMFR	2,4,6,8,10,12	minutes
Resin Radius	FBR, CMFR	0.1,0.4,0.8,1.2	mm
Average Resin Attrition	FBR	0,5,10,15	% of loss
Frequency of Resin Cleaning/Maintenance	FBR	0,3,6,9,12	Frequency in years
Regeneration Ratio	CMFR	5,10,15,20,25	%
Resin Volume Concentration in IX Reactor	CMFR	10,20,30,40,50	(ml resin) / (L reactor volume)
Resin Volume Concentration in Regeneration Reactor	CMFR	50,100,150,200,250,300	(ml resin) / (L reactor volume)
Flow Rate Capacity	FBR, CMFR	1	MGD
Average Flow Rate	FBR, CMFR	0.5	MGD

3.2.2.2 Genetic Algorithm

An alternative method for running the code was developed using a simplified genetic algorithm (GA). This method can be used to determine an optimal design scenario, given a range of input options, without having to compute all possible permutations. GAs are stochastic optimization algorithms that emulate Darwinian evolution in order to find a global solution to optimization problems (Goldberg, 1989). Therefore, GAs represent a suitable optimization method for the integrated model. The GA can perform single objective optimization for either environmental impact or cost.

The structure of utilizing the model using a GA is shown in Figure 3.2. The simplified GA generates a population of random inputs to the model. Subsequently, it cycles through a number of generations by: running the model with the population of inputs, evaluating the result, removing a certain percentage of the options that are farthest from the target parameter (either environmental impact or cost) by using a selectivity parameter, and performing random mutations of the inputs before cycling through the next generation. This allows the initial population to be culled successively until a more optimal result is obtained. The possible initial parameters can also be limited to certain set. For example, if certain design parameters are constrained, the GA can find the optimal choice within those constraints.

For the purpose of testing the GA, it was run using the same possible permutations of input options shown in Table 3.1, but the reactor type was assumed to only be a CMFR. This provides a total number of possible permutations of 7,200. The parameter being optimized was the normalized lifetime cost of the system. The initial population was tested at 100, 50, and 20. A selectivity of 100% was used, meaning that all of the population that has a normalized lifetime cost above the average of the total population is removed in every generation. The mutation rate was also set at 20%. This indicates that 20% of the inputs will be randomly modified to increase or decrease. This process is continued until a single design scenario remains as the solution. This simplified GA lacks some conventional GA components, such as a crossover rate; however, the simplified approach reduces complexity of the code while still achieving satisfactory results.

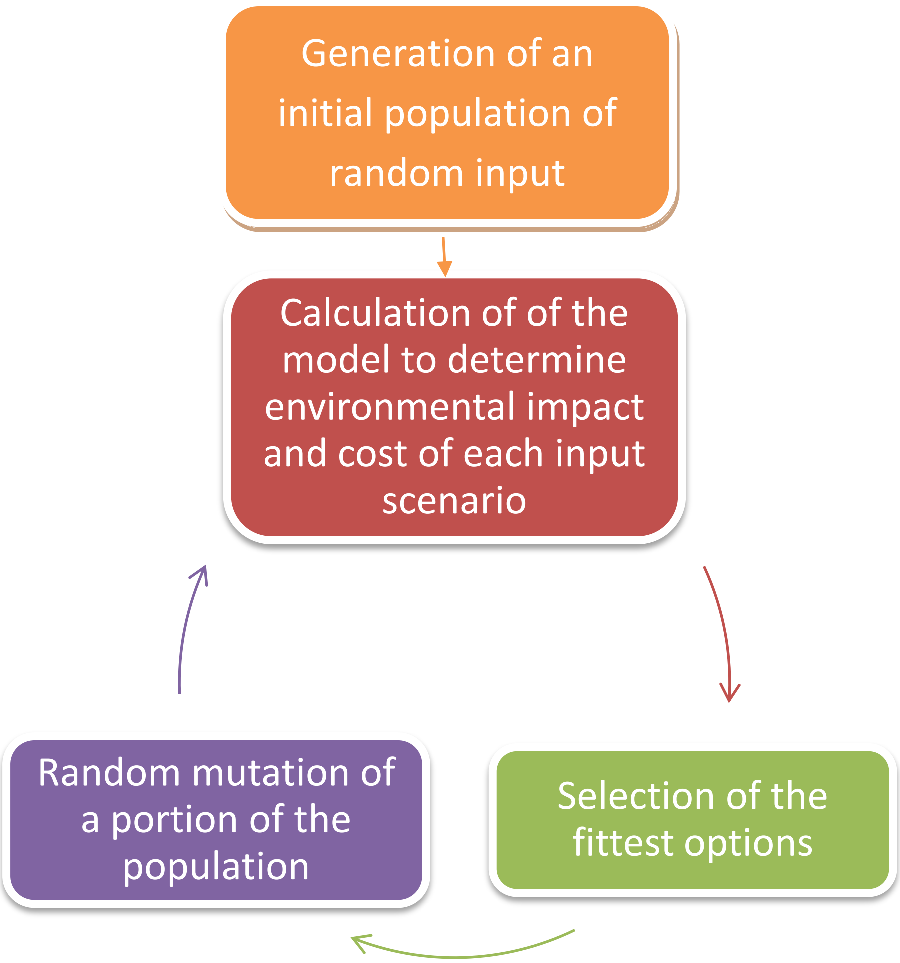

Figure 3.2: Model utilization structure with genetic algorithm

3.2.3 Life Cycle Assessment Methods

The LCA performed in the model follows the same method as described in Amini et al. (2015) for IX systems. The LCA focuses primarily on the operation phase, because this was found to have the most significant impact over the life cycle of the system (Amini et al., 2015). The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI 2.1) (Bare et al., 2003) method in Simapro 8.0.3 was used for the life cycle impact assessment (LCIA) because it is suitable for North America. The results are presented in ten impact categories that include ozone depletion, global warming, acidification, eutrophication, eco-toxicity, smog formation, human health carcinogenics, human health non-carcinogenics, human health criteria pollutants, and fossil fuel use. A single score was also calculated to allow for easier comparison among systems and impact contributors using normalization values for North America (Bare et al., 2006), which were aggregated using equal weighting. The functional unit is 1 million gallons of treated per day with a removal of 1 mg/L dissolved organic carbon (DOC) over a period of 20 years, which is the lifetime of the CMFR systems.

3.2.4 Life Cycle Cost Analysis Methods

The LCCA follows the methods described in Amini et al. (2015) for calculation of costs for the operation phase of IX systems, using net present value (NPV). Capital expenses (CAPEX) are also estimated in the system, utilizing a simple cost curve developed from capital costs for several IX systems obtained from system manufacturers. Capital costs can vary widely depending on location or other design-specific considerations; therefore, CAPEX is only a general estimate. The model, however, estimates differences in the CAPEX based on design considerations. For example, a larger HRT within the system will require a larger IX reactor volume. The capital cost increase of this change in volume is accounted for in the model. All cost calculation results are presented in 2017 dollars.

3.2.5 Method for Assessing Impacts of Brine Waste Treatment

Disposal or treatment of the waste brine that is generated by IX is one of the environmental concerns of IX treatment. Amini et al. (2015) found that the primary method for dealing with the waste brine from IX systems studied was to discharge the waste to the wastewater treatment plant (WWTP). Waste brine can adversely affect wastewater treatment plant operation, particularly when biological processes are utilized (Maul et al., 2014; Panswad and Anan, 1999). However, there are currently few methods to take into account the environmental impact of such treatment. Amini et al. (2015) took into account the increased environmental impact due to the treatment of higher volumes at the WWTP. However, a method is needed to better quantify the effects of the brine on WWTP operation. To better account for the impact, a method has been developed and incorporated into the model that accounts for the increase environmental impacts and costs in WWTPs that have activated sludge, nitrification, and denitrification processes.

This method takes into account the effect of an increase of ionic strength in the wastewater on the reaction rate of the WWTP operations when NaCl is used as the regenerant. The model includes NaCl and $NaHCO_3$ as possible regenerants; however, the effect of HCO_3^- on WWTP operation is not expected to be as significant and is not currently evaluated. The model currently assumes the WWTP plant flow to be approximately equal to average water treatment plant flow, although in reality, the WWTP flow may vary depending on collection system design and regional inflow and infiltration rates. The waste brine volume and concentration are calculated in the model and the dilution of this volume with typical WWTP flow is calculated for a daily basis. The typical total dissolved solids (TDS) for medium strength wastewater is assumed at 500 mg/l (Tchobanoglous et al., 2003). The ionic strength is calculated using equation 1 (Tchobanoglous et al., 2003).

$$I = (2.5 \times 10^{-5})(TDS) \tag{1}$$

The Davies equation (Crittenden & MWH, 2012) was used to calculate the change in the activity coefficient, shown in equation 2.

$$log_{10}\gamma_{\mathrm{i}} = -AZ_i^2\left(\frac{I^{\frac{1}{2}}}{1+I^{\frac{1}{2}}} - 0.3I\right) \tag{2}$$

where A is a constant (assumed 0.5 for 15°C), γ_i = activity coefficient for ionic species, I = ionic strength of solution, mol/L(M), Zi = number of replaceable hydrogen atoms or their equivalent (for oxidation–reduction reactions, Z is equal to the change in valence). The increase in activity coefficient is calculated, which affects the reaction rate using kinetics as shown in equations 3 for the example of nitrification.

$$r_A = -\mu_{max} \frac{\{NH_4{}^+\}}{K_{S,NH_4{}^+} + \{NH_4{}^+\}} \frac{\{O_2\}}{K_{S,O2} + \{O_2\}} X_{AOB} \tag{3}$$

where r_A=denitrification rate, mg/L·d, μ_{max}=maximum specific growth rate constant, d^{-1}, K_S=half saturation constant, mg/L, $\{NH_4{}^+\}$=activity (effective concentration) of ammonium, mg/L, $\{O_2\}$=activity (effective concentration) of dissolved oxygen, mg/L, X_{AOB}=concentration of ammonium oxidizing bacteria, mg/L

The change in activity coefficient will affect the effective concentration of ammonium ($\{NH_4{}^+\}$) and dissolved oxygen ($\{O_2\}$), and microbial activity of nitrifying bacteria. In this study, it is assumed that the change will proportionally affect the oxygen needed for BOD degradation and nitrification as well as the amount of electron donor to achieve the same rate of denitrification. In the model, this is taken into account as a proportional increase in electricity requirements for aeration as well as methanol requirements, which can incur costs as well as environmental impacts. The assumed typical aeration rates and costs for this assessment are included in the supporting information (Table S.1).

The brine received at the WWTP can also cause other issues for its operation as well as cost. The brine will increase the conductivity of treated wastewater at the WWTP. These sources of conductivity can possibly become higher than permitted limits for the WWTP. Therefore, proper permitting requirements must be taken into account when considering IX implementation. Furthermore, increases in conductivity can decrease settleability of solids (Tchobanoglous et al., 2003), which can require a larger clarifier that incurs higher costs. Furthermore, higher conductivity can decrease the solubility of dissolved oxygen, requiring higher aeration rates (Wilde & Radtke, 2006). A rise in the brine concentration of wastewater effluent can also restrict its use in agriculture due to its ability to cause sodic soil and a variety of negative effects on crops, such as necrosis of the plants (Bernstein, 1975). Furthermore, discharge of wastes with high NaCl concentrations to receiving waters can have adverse effects on their associated ecosystems (Canedo-Arguelles, 2013). These considerations are not taken into account in the current model, but can be added to the model in the future to provide a more robust assessment.

3.3 Results

3.3.1 Evaluating Trends

The results from the 12,000 possible permutations were calculated with the model and trends in the effects of various design choices on the environmental impacts and costs over the lifetime of the system were evaluated. The average lifetime cost (NPV) and average environmental impact, normalized by the functional unit, were calculated for the inputs options of each decision variable. These results show general trends among all scenarios but cannot be used to create rules of thumb that can be used in every situation. Therefore, although these show the general effects of design choices, each design scenario must be evaluated individually to obtain context appropriate results. These results show that overall FBR systems tend to have lower environmental impact and cost than CMFR systems, as shown in Figure 3.3. However, maintenance of the resins in FBR systems is very important to reducing environmental impacts compared to CMFR systems. If the resins are not maintained regularly, such as with NaOH cleaning, the regeneration rate of FBR systems increases significantly, increasing its environmental impact compared to CMFR systems. The effect of resin cleaning frequency is shown in Figure 3.4. This is consistent with findings in Amini et al. (2015). Resin loss can also have a significant effect on FBR systems and higher resin loss tends to incur higher costs and environmental impacts.

The choice of regenerant also had significant impact on the environmental impacts and costs, as shown in Figure 3.5. Maul et al. (2014) compared various IX regenerants, including NaCl and $NaHCO_3$, and found that based on raw material extraction and production of the salt, NaCl has lower costs and environmental impacts than using $NaHCO_3$ as a regenerant. This is because much higher quantities of $NaHCO_3$ are needed to achieve the same regeneration efficiency. In addition to the production of the salt, the model used in this research takes into account the increased costs and environmental impacts on the WWTP by waste brine treatment. However, even with the additional costs and impacts of treatment due to NaCl, it still tends to incur lower environmental and cost than $NaHCO_3$.

Choice of resin size appears to also affect the impacts and costs, as shown in Figure 3.6. Larger resin sizes appear to have higher lifetime impacts and costs. This is likely due to the decrease in surface area, which can decrease IX capacity of the resin. This decreased capacity therefore requires more frequent regeneration, which utilizes more salt and creates more brine waste. However, utilizing small resin sizes in IX systems can introduce issues in operation and maintenance. For example, smaller resin sizes can possibly increase the potential for unintentional resin attrition in FBR systems and can increase the already high resin attrition rate of CMFR systems. Furthermore, it can introduce problems with resin settling. Therefore, although lower resin sizes are preferred, this must be balanced with possible resin attrition.

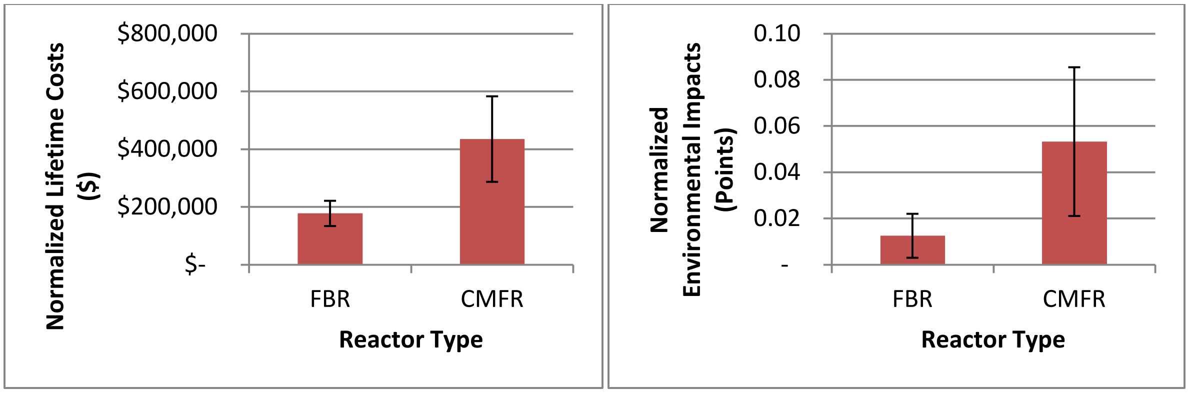

Figure 3.3: Trend of costs and impacts for FBR vs CMFR systems

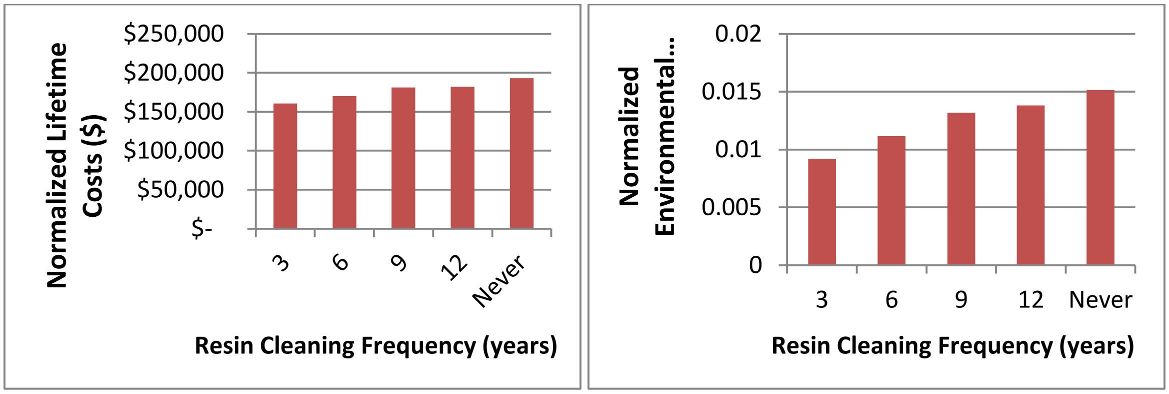

Figure 3.4: Trend of costs and impacts for rein cleaning frequency

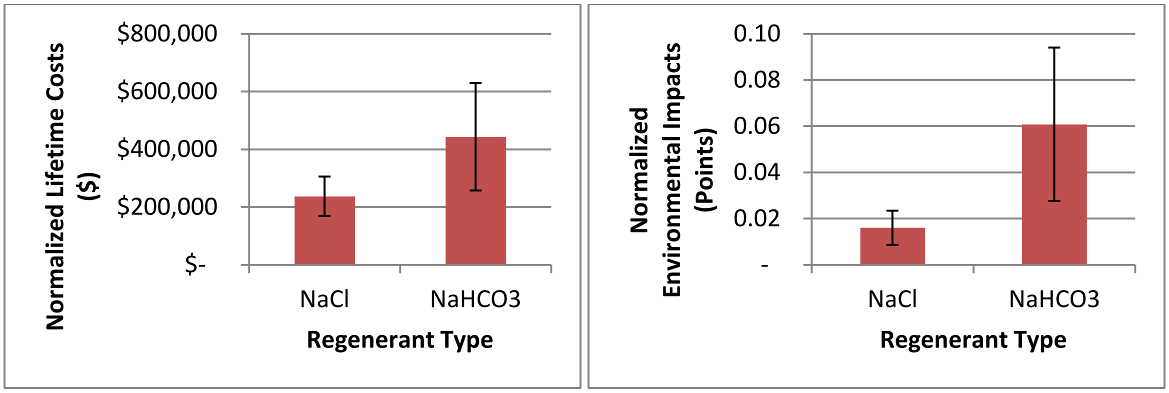

Figure 3.5: Trend of costs and impacts for NaCl vs NaHCO$_3$ regenerants

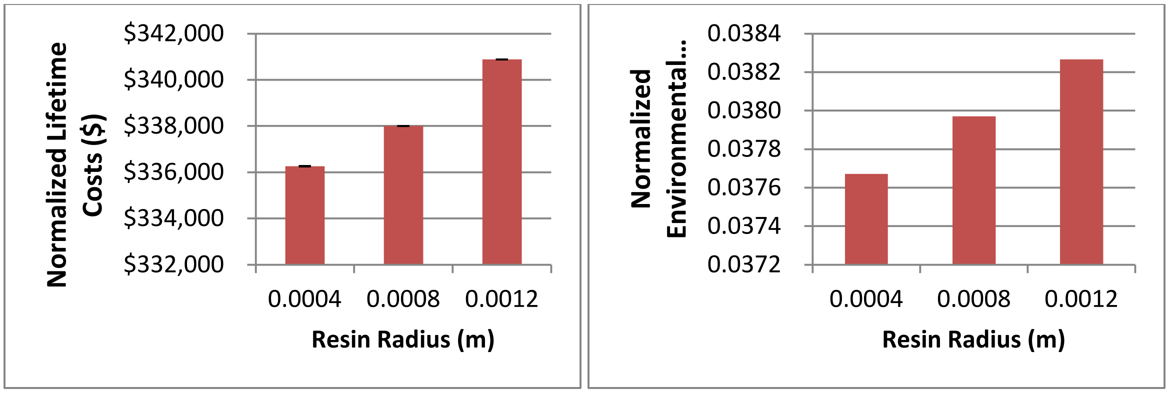

Figure 3.6: Trend of costs and impacts for various resin sizes

HRT is one of the key design parameters of the system. The results show that higher HRTs tend to incur lower cost and environmental impact overall, as shown in Figure 3.7. This is likely because the increase in HRT can improve IX contact time and decrease regeneration requirements, even though a larger reactor volume is required. Therefore, the operation impacts and costs appear to outweigh the increased capital requirements. However, the when the HRT reaches above 10 minutes, the reactor size gets to a size that requires a different type of construction. Smaller systems can be effectively build with prefabricated units, but larger systems must generally be built on site with concrete tanks, which can incur significantly higher cost and impacts. Therefore, choosing HRTs that are approximately 8-10 minutes provide the lowest impact and cost. This is however context sensitive to the flow rate included in this assessment. In general, the results indicate that larger HRTs are preferable if a larger reactor does not incur significantly higher costs, such as a transition from prefabrication to on-site construction.

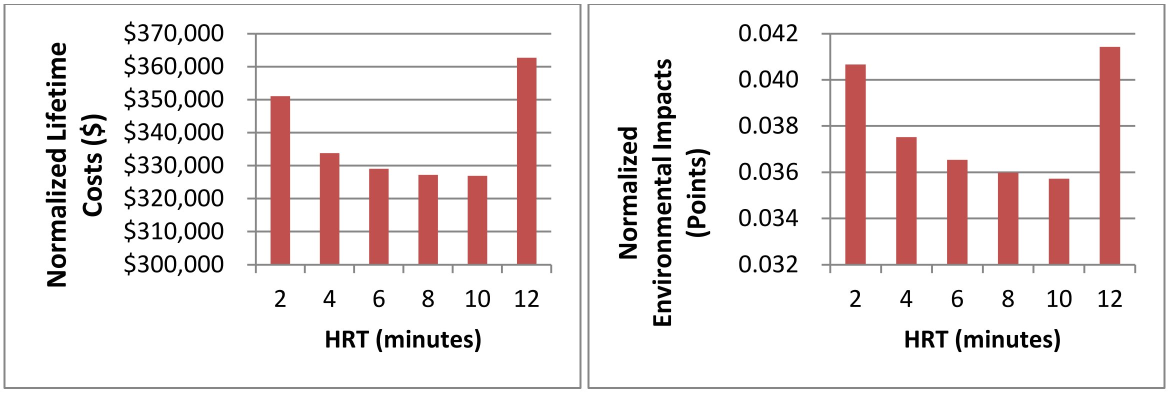

Figure 3.7: Trend of costs and impacts for various HRTs

The regeneration ratio, resin concentration in the IX reactor, and resin concentration in the regeneration reactor are key design parameters for CMFR systems. The results of these three parameters are shown in Figure 3.8-3.10 below. Regeneration ratio controls how much of the resin is regenerated in each cycle. Larger regeneration ratios will increase the size of regeneration reactors in order to maintain the same resin concentration in the regeneration reactor. The larger reactors can incur a higher cost, but the higher regeneration ratio would also improve removal efficiencies in the IX reactor. Like regeneration ratio, a higher concentration of resin in the IX reactor and regeneration reactor can reduce the size and capital costs of the reactor, but can decrease IX removal efficiency or regeneration efficiency. Overall, these effects appear to creating small differences between various choices for both environmental impact and cost. At most, a normalized lifetime savings of $10,000 can be achieved. A higher regeneration ratio can achieve lower costs, but also incurs higher environmental impact. Therefore, a regeneration ratio of approximately 15% can reduce both. Therefore, choices regarding these three design parameters may be made based on other site specific considerations. For example, a choice of a smaller regeneration ratio and higher concentrations in the IX reactor and regeneration reactor may be preferable overall to reduce footprint of the system and reduce space requirements. For the concentration of resin in the IX reactor, a higher resin concentration incurs lower cost and impact, likely due to decrease reactor costs. However, for the resin concentration in the regeneration reactor, a lower concentration is preferable, which likely improve the regeneration efficiency and reduces salt consumption.

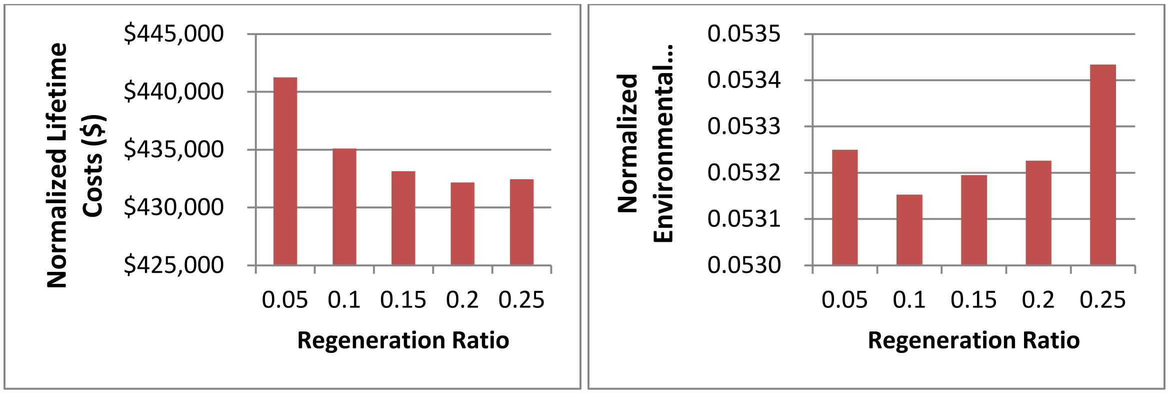

Figure 3.8: Trend of costs and impacts for various regeneration ratios

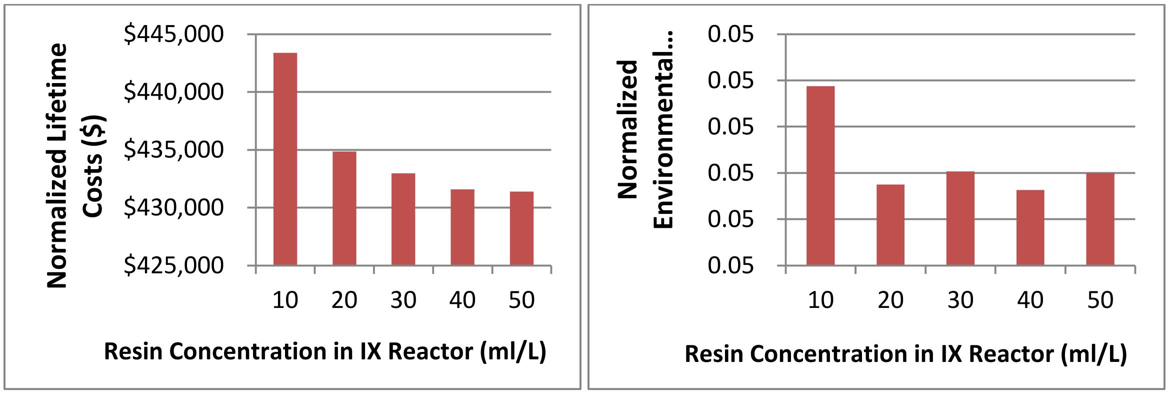

Figure 3.9: Trend of costs and impacts for various resin concentrations in the IX reactor

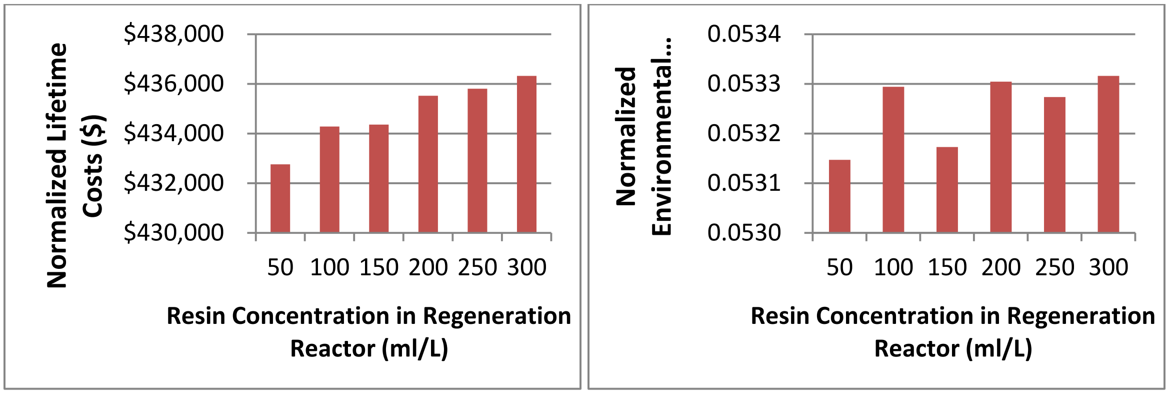

Figure 3.10: Trend of costs and impacts for various resin concentrations in the regeneration reactor

3.3.2 Genetic Algorithm

The genetic algorithm was tested with 7,200 permutations using several initial population sizes. This was then compared to results of all the possible permutations to evaluate how accurate the GA can be. At least five tests were performed at each initial population of 100, 50, and 20. The true optimal solution and the true worst solution had a difference of 125%. In all of the tests, however, the GA was able to identify solutions within 2% of the true optimum and in most cases was within 0.5% of the true optimum. Increasing the initial population size from 20 to 100 appeared to have some effect on more consistently producing results with a lower error. When an initial population size of 100, 50, and 20 were used, approximately 60%, 50%, and 40% of the results, respectively, were within 0.5% of the true optimum. This difference, however, is quite small since all of the results were within 2% of the true optimum. The GA can also save significant time for calculation. The number of runs required to achieve a final result was found to approximately be twice the initial population. Therefore, with an initial population of 20, a result that is within 2% of the true optimum can be identified with approximately 40 code runs instead of 7,200. This means that utilizing the GA to find an optimal result can reduce the run time by approximately 99%.

3.3.3 Brine Waste Treatment

The impact and cost of treating the brine waste at the WWTP was calculated for all of the scenarios. This takes into account the increased electricity requirements for aeration of activated sludge and nitrification processes as well as the increase in carbon source requirements for denitrification.

The cost associated with brine water treatment will not be incurred at the water treatment plant (WTP), but at the WWTP. In locations where they are separate entities, the WTP may not be responsible for these costs; however, in this analysis these costs are included in the overall cost of the system to give perspective regarding the effects of creating more brine waste in IX systems.

Overall, both the costs and environmental impacts of brine waste treatment tend to be approximately 7-20% of the total costs and impacts. Therefore, increases in brine waste can contribute significantly toward decreasing the overall sustainability of IX systems. However, when they sent to a WWTP for treatment, they do not outweigh other contributors to environmental impacts and costs, such as electricity, resin, and salt usage which contribute significantly to the overall impacts and costs.

3.4 Conclusions and Recommendations

Overall, the general trends indicate that designing an IX system with an FBR configuration, NaCl as a regenerant, lower resin sizes, and higher HRTs (if a larger reactor does not incur significantly higher costs) can reduce the environmental impacts and costs of IX systems. For FBR systems in particular, regular resin cleaning every 3 years in FBR systems and low resin attrition can also provide the most benefit. For CMFR systems, regeneration ratios of approximately 15%, high resin concentrations in the IX reactor, and lower resin concentrations in the regeneration reactor can provide the lowest costs and impact. These trends, however, do not apply to every situation. Site specific design considerations and other constraints can affect the system and particular scenarios can be evaluated with the model to identify optimal options. Furthermore, taking into account the effect of the brine on biological processes at the WWTP can contribute to approximately 7-20% of lifetime impacts and costs of IX systems.

Future research that can improve upon the current work includes incorporation of IX systems that remove other types of contaminants. In addition, the current model can be adapted to be more accessible to water professionals so that it can be used as a tool for learning and estimation of the sustainability of various design scenarios. This can take the form of a user-friendly software tool for evaluating design scenarios.

3.5 Acknowledgements

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3.6 References

Azapagic, A., 1999. Life cycle assessment and its application to process selection, design and optimisation. *Chemical Engineering Journal, 73*(1), 1-21. doi:10.1016/s1385-8947(99)00042-x

Azapagic, A., Millington, A., & Collett, A., 2006. A Methodology for Integrating Sustainability Considerations into Process Design. *Chemical Engineering Research and Design, 84*(6), 439-452. doi:10.1205/cherd05007

Bare, J. C., Norris, G. A., Pennington, D. W., McKone, T., 2003. TRACI – The Tool for the Reduction and Assessment of Chemical and other Environmental Impacts. Journal of Industrial Ecology. 6, 49-78.

Bare, J., Gloria, T., Norris, G., 2006. Development of the Method and U.S. Normalization Database for Life Cycle Impact Assessment and Sustainability Metrics. Environmental Science and Technology. 40, 5108-5115.

Bernstein, L. (1975). Effects Of Salinity And Sodicity On Plant Growth. Annual Review of Phytopathology, 295-312.

Canedo-Arguelles, M., Kefford, B.J., Piscart, C., Prat, N., Schafer, R.B., Schulz, C.J., (2013). Salinisation of rivers: An urgent ecological issue. Environmental Pollution. 173, 157-167.

CDM, 2007. Evaluation of Methanol Feed, Storage and Handling Costs at Municipal Wastewater Treatment Facilities (Rep).

Choe, J.K., Mehnert, M., Guest, J., Strathmann, T.J., Werth, C.J., 2013. Comparative assessment of the environmental sustainability of existing and emerging perchlorate treatment technologies for drinking water. Environ. Sci. Technol. 47, 4644-4652.

Crittenden, J. C., & MWH., 2012. MWH's water treatment: Principles and design. Hoboken, N.J: Wiley.

Dominguez-Ramos, A., Chavan, K., García, V., Jimeno, G., Albo, J., Marathe, K.V., Yadav, G.D., Irabien, A., 2014. Arsenic removal from natural waters by adsorption or ion exchange: an environmental sustainability assessment. Ind. Eng. Chem. Res. 53, 18920-18927.

Environmental Dynamics International, 2011. Aeration Efficiency Guide. Columbia, MO.

Fazeni, K., Lindorfer, J., & Prammer, H., 2014. Methodological advancements in Life Cycle Process Design: A preliminary outlook. *Resources, Conservation and Recycling, 92,* 66-77. doi:10.1016/j.resconrec.2014.08.011

Hu, Y. & Boyer, T., 2017. Integrated bicarbonate-form ion exchange treatment and regeneration for DOC removal: Model development and pilot plant study. Water Research, 115, 40-49. doi:10.1016/j.watres.2017.02.013

Maul, G., Kim, Y., Amini, A., Zhang, Q., Boyer, T., 2014. Efficiency and Life Cycle Environmental Impacts of Ion-exchange Regeneration Using Sodium, Potassium, Chloride, and Bicarbonate Salts. Chemical Engineering Journal. 254, 198-209.

Ras, C., von Blottnitz, H., 2012. A comparative life cycle assessment of process water treatment technologies at the Secunda industrial complex, South Africa. Water SA 38, 549-554.

Tchobanoglous, G., Burton, F. L., Stensel, H. D., & Metcalf & Eddy., 2003. Wastewater engineering: Treatment and reuse. Boston: McGraw-Hill.

Vince, F., Marechal, F., Aoustin, E., & Bréant, P., 2008. Multi-objective optimization of RO desalination plants. *Desalination, 222*(1-3), 96-118. doi:10.1016/j.desal.2007.02.064

Vorosmarty, C. J., Green, P., Salisbury, J., & Lammers, R., 2000. Global Water Resources: Vulnerability from Climate Change and Population Growth. Science, 289(5477), 284-288. doi:10.1126/science.289.5477.284

Wilde, F. D., & Radtke, D. B. (2006). *Handbooks for water-resources investigations*. Washington, D.C.: U.S. G.P.O.

Zhang, J., Amini, A., O'neal, J. A., Boyer, T. H., & Zhang, Q., 2015. Development and validation of a novel modeling framework integrating ion exchange and resin regeneration for water treatment. Water Research, 84, 255-265. doi:10.1016/j.watres.2015.07.027

3.7 Supporting Information

Table 3.2: Waste brine treatment, typical assumed values

Item	Amount	Units
Activated sludge typical electricity requirements	3,954	kWh/MG
Fine bubble diffuser aeration rate	1.6	kg O_2/kWh
Nitrification air requirements	4.6	kg O_2/kg TKN
TKN for medium strength wastewater	35	mg/L
Typical concentration of nitrate after nitrification	17	mg/L
Methanol requirement	1.91	mg /mg nitrate
Methanol cost	1.5	$/gallon
Electricity cost	9	cents/kWh
Sources: (CDM, 2007; Environmental Dynamics International, 2011; Crittenden & MWH, 2012; Tchobanoglous et al., 2003)		

Chapter 4: Life Cycle Environmental Impact and Cost Evaluation of Combined Cation/Anion Exchange Systems for Small Potable Water Systems (Task 3)

4.1 Introduction

Small potable water systems (PWS) comprise the majority of all PWS, yet they often face significant economic and environmental challenges in financing, operating, and maintaining their systems (USEPA, 2013). The USEPA has therefore highlighted the need these PWS have for technologies that can meet their operational challenges while reducing economic and environmental impacts. Ion exchange (IX) is a treatment technology that is gaining traction among small PWS and has been shown to have economic and environmental advantages over alternative technologies (Ras and von Blottnitz, 2012; Dominguez-Ramos et al., 2014).

IX systems can be used to remove a wide range of contaminants and generally focus on a single target contaminant, either a cation or anion. When removal of multiple contaminants is required, often more than one type of IX system must be implemented. For example, to remove natural organic matter (NOM) and hardness, separate IX systems can be implemented to individually remove the respective target contaminants. However, implementing multiple systems adds complexity, infrastructure, and operating expenses to water treatment plants. Combined cation/anion exchange (CCAE) is a viable method of removing multiple contaminants in a single unit process, but CCAE has rarely been investigated in the context of drinking water treatment.

Apell and Boyer (2010) were the first to investigate CCAE for drinking water treatment to remove dissolved organic matter (DOM) and hardness, demonstrating the viability of the system. Further studies have also investigated the interactions of Na^+, $Mg^{2+,}$ Ca^{2+}, Cl^-, HCO^-_3 , SO^{2-}_4 , and DOM during combined ion exchange (Indarawis and Boyer, 2013), improved methods for removal of DOM and hardness (Comstock and Boyer, 2014), and removal of heavy metals (Cu(II), Ni(II)) and tannic acid (Fu et al., 2015). Such systems can achieve removal efficiencies of greater than 75% and in most cases greater than 90%. Furthermore, combined IX has the ability to achieve superior performance compared to the alternative conventional treatment. For example, Comstock and Boyer (2014) found that combined IX achieved greater reductions in DOM and hardness than either coagulation or precipitative softening.

Implementing cation and anion exchange in a single process has the potential to reduce infrastructure requirements, energy usage, and chemical needs, which can have significant implications in terms of costs and environmental impacts. For instance, salt usage and brine waste treatment can greatly contribute to environmental impacts and costs for water treatment plants (WTPs) that use IX as well as and wastewater treatment plants (WWTPs) that receive their waste (Amini et al., 2015; Maul et al., 2014; Panswad and Anan, 1999). Conventional anion exchange uses a regenerant such as NaCl, but only the Cl^- ion is utilized in the anion regeneration process, while the Na^+ becomes waste. CCAE can potentially cut the salt requirements as well as brine waste production by utilizing both the cation and anion of the regenerant. No studies, however, have investigated the life cycle economic and environmental benefits of CCAE.

The purpose of this paper is to quantify the life cycle environmental impact and cost benefits of CCAE, as well as to identify opportunities for improvement of CCAE. It is hypothesized that the benefits provided by CCAE, as described above, can translate into lower environmental impacts, lower construction costs, and lower operating costs than conventionally separate IX systems. CCAE systems are currently uncommon in small PWS. Therefore, there is high potential for implementing such systems to provide great benefit to small PWS.

4.2 Materials and Methods

In order to compare the environmental impacts and costs, this study performs a life cycle assessment (LCA) and life cycle cost analysis (LCCA), following the International Organization for Standardization (ISO) methodological framework for environmental impact Assessment (ISO, 2006a, 2006b). This includes Goal and Scope Definition, Inventory Analysis, Impact Assessment, and Interpretation.

4.2.1 Goal and Scope

The goal of this study is to quantify the life cycle environmental impacts and life cycle costs of CCAE in potable water systems and identify opportunities for improvement. Furthermore, these impacts and costs will be compared with more conventional separate IX systems. This provides industry valuable insight into the benefits and drawbacks of CCAE technology in terms of the cost and environmental impacts. Furthermore, as the first LCA on CCAE for potable water systems, it encourages further study into novel IX design configurations that can improve environmental and economic sustainability.

4.2.1.1 System Boundary

The system boundary of the LCA focuses primarily on the operation phase of the IX system. This is because previous studies found the construction phase to contribute relatively little to environmental impact of IX systems over the life cycle (Choe et al., 2013; Amini et al., 2015). The LCA system boundary therefore includes raw material extraction, production, transportation, and use. Pretreatment and post-treatment that are employed in the treatment plant but that are not necessary to the operation of the IX system are not included in the system boundary.

4.2.2 System Descriptions

This study evaluates and compares CCAE to four separate IX system scenarios, as shown in Table 4.1. The systems are all designed to remove DOC and hardness from groundwater. IX systems are typically designed with either a fixed bed reactor (FBR) or a completely mixed flow reactor (CMFR) (Amini et al., 2015). For separate IX, two contactor reactors are required, through which the raw water flows in series. When both anion and cation exchange is required is required, these two types of reactors can be utilized together in four possible combinations. The FBR systems perform discrete regeneration within the contactor, while CMFR systems send the resin to a separate tank for regeneration. Fresh brine is used for each resin regeneration. Therefore, in these systems, Na^+ is used for cation regeneration, creating a waste of Cl^- and hardness, while Cl^- is used for anion regeneration, creating a waste of Na^+ and DOC. Diagrams showing the four system configurations of separate IX are provided in the Supporting Information (Figures 4.6-4.9).

The CMFR and FBR systems for DOC removal are based on data from Amini et al. (2015) as described in Chapters 2 and 3. The FBR softening system is based on data from a treatment plant in Florida that performed IX softening. This plant has a 4 MGD capacity, average flow of 1.25 MGD, total influent hardness of approximately 275 mg/L, and effluent hardness of approximately 65 mg/L (210 mg/L removal). To the author’s best knowledge, there is currently no known CMFR softening system (IXOM manufacturer confirmed no existing systems). Therefore, this system is primarily theoretical and is based on design characteristics and parameters provided by the manufacturer. Further methods for data collection for these four scenarios are described in Section 4.2.3 and 4.2.4.

The CCAE system scenario is based on a small water treatment plant in Florida, constructed in 2015. To the author's best knowledge, it is the first CCAE drinking water treatment system in the United States and is constructed by Ixom (formerly Orica Chemicals). The system uses the proprietary magnetically enhanced resin called MIEX. The commercial name of the Ixom's CCAE system is MiCO, which stands for MIEX co-removal. The system has a treatment capacity of 1 million gallons per day (MGD), an average flow of 0.33 MGD, and has groundwater as the source water. The influent total hardness is approximately 340 mg/L and effluent hardness is approximately 130 mg/L (approximate removal of 210 mg/L). The influent DOC concentration is estimated at 5.18 mg/L influent and 2.48 mg/L effluent. This is based on the both color and UV_{254} data provided by the treatment plant. These were converted to DOC in mg/L using regression equations found in Amini et al. (2015) and were averaged. The system employs a single CMFR reactor in which both cation and anion exchange is performed. A diagram of the CCAE system configuration is shown in Figure 4.1 below.

Currently, however, the treatment plant is not operated to employ all of the potential benefits of CCAE technology. For example, during regeneration CCAE has the potential to use the same brine for both cation and anion regeneration by allowing for the use of both Na^+ and Cl^-, potentially dramatically reducing salt requirements and brine waste generation while also reducing the Na^+ and Cl^- concentrations in the spent brine. However, the real plant currently only uses fresh brine and is not taking advantage of this potential design feature. Due to such differences, another scenario is also included in the analysis, which takes into account a more idealized CCAE scenario. The theoretical scenario uses the same system design as the actual system but uses the same brine for cation and anion regeneration at an assumed 80% regeneration efficiency and employs pumps that are equivalent in size to the CMFR systems used in the other scenarios.

Table 4.1: Configuration scenarios compared in this study for the removal of DOC and hardness from groundwater

Scenario:	1	2	3	4	5	6
Anion Exchange	CCAE (Theoretical)	CCAE (Actual)	FBR	FBR	CMFR	CMFR
Cation Exchange			FBR	CMFR	FBR	CMFR

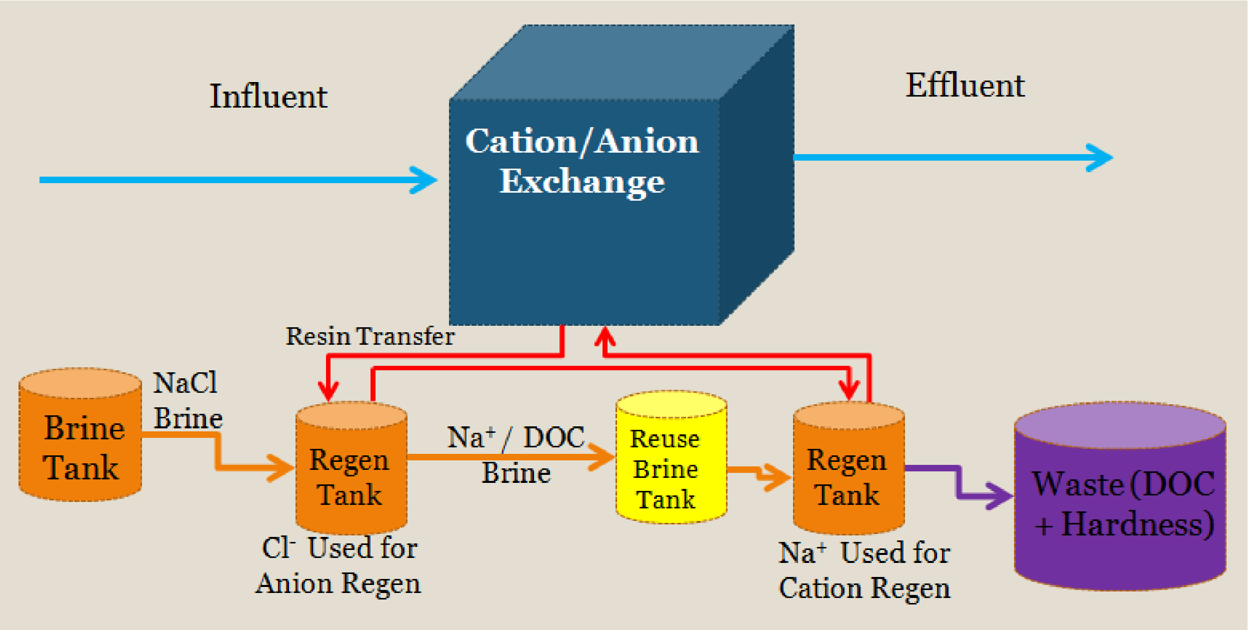


Figure 4.1: Combined cation/ anion exchange (CCAE) system configuration with regeneration

4.2.3 Life Cycle Inventory Methods

The data to develop the life cycle inventory (LCI) is based on data collected through visits to the CCAE water treatment plant as well as eight other drinking water plants in Florida that implement separate IX (Amini et al., 2015), consulting engineering and manufacturers of the systems, evaluating recorded plant operation data, and by consulting with plant operators. All of the treatment plants that employ separate IX are designed to remove DOC and some are designed for softening. This data was used to generate an LCI for hypothetical systems that match the size and treatment performance of the real CCAE treatment plant.

The LCI focuses on the operation phase, as discussed above. Foreground data, which refers to inventory data specific to the system studied, include resin usage, electricity usage, salt usage, brine waste treatment, chemical usage. This is consistent with previous studies (Ras and von Blottnitz, 2012; Choe et al., 2013; Amini et al., 2015). Background data refers to generic or average data typically found in databases or literature. These were obtained from Ecoinvent 3 and USLCI databases, available in Simapro version 8.0.3.

The LCI for separate IX systems was also generated with data based on system manuals, engineering specifications, and averaged inventory data. In particular, the LCI for both the FBR and CMFR systems for DOC removal were obtained using the methods and model described in Chapter 3. The resin size, HRT, and other design inputs are based on average values for the real installations studied in Amini et al. (2015). However, the systems are assumed to be operated in an ideal but realistic manner. Therefore, operational parameters such as the frequency of resin cleaning, were set at conditions that do not incur unnecessarily high impacts and costs (e.g. resin cleaning every 3 years). Furthermore, the LCI for the FBR softening system was collected using the methods described in Amini et al. (2015). The data for the CMFR softening system, however, is based on design parameters provided by the manufacturer. These data were normalized to match the flow characteristics and contaminant removal of the CCAE system which has an average flow of 0.33 MGD, total hardness removal of approximately 210 mg/L, and DOC removal of approximately 2.7 mg/L. A time period of 20 years is used for the LCI because this is the approximate design life of the CCAE system and other CMFR systems (the design life of the fixed bed systems is approximately 30 years).

4.2.4 Life Cycle Impact Assessment Methods

The life cycle impact assessment (LCIA) was carried out using the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI 2.1) (Bare et al., 2003), which uses assessment methods suitable for North America. This evaluates environmental impact in ten impact categories, including ozone depletion, global warming, acidification, eutrophication, eco-toxicity, smog formation, human health carcinogenics, human health non-carcinogenics, human health criteria pollutants, and fossil fuel use. A single score of environmental impact was obtained by normalizing the results using normalization values for North America found in Bare et al. (2006). These were aggregated using equal weighting among all categories to obtain environmental impact points. A time period of 20 years is also used for the LCIA.

For this analysis, the cost and environmental impact of brine waste was taken into account using the same method described in Chapter 3. Therefore, it assumes discharge of the brine waste to a WWTP, which is the most common method of brine disposal, and assumes the WWTP and WTP to be approximately the same size. It takes into account treatment of the volume of waste at a typical WWTP (based on Ecoinvent data). Furthermore, it takes into account an increase in costs and environmental impacts based on the potentially higher aeration and carbon requirements for an activated sludge system with nitrification and denitrification, due to the increase in ionic strength caused by the brine, which decreases the reaction rate constant.

4.2.5 Life Cycle Cost Analysis Methods

A LCCA was performed on the same system studied in the LCA. Estimated costs of the construction phase are also included in the LCCA. The operating expenses (OPEX) are based on data that were collected and calculated using information from literature as well as plant operators and managers, and engineering manufacturers. Calculation of OPEX, such as salt usage and resin usage, are based on LCI data. Individual cost items, such as the cost of salt per ton, were set to match costs reported by the CCAE system to provide a fair comparison. Cost of labor was not included in the scope of the analysis. Furthermore, the cost of salt and resin includes the cost of transport.

The OPEX was calculated using the present value method by multiplying annual operating costs by a uniform present value (UPV) factor. The UPV was calculated using Equation (1), with an interest rate (i) of 5% for a lifetime (n) of 20 years (the approximate design life of the CCAE and CMFR systems). Using a UPV assumes that the annual operating costs are constant in the study period. For energy cost, a non-uniform present value (UPV*) was calculated using Equation (2). The Energy Efficiency and Renewable Energy (EERC) program (version 2.0-15) from the U.S. Department of Energy was used to calculate the annual energy escalation rate (e) of 0.76% for Florida, with a default carbon price. All cost calculation results are presented in 2017 dollars.

The capital expenses (CAPEX) of the CCAE system are a general estimate based on data provided by the treatment plant and manufacturer. The CAPEX of the separate IX systems were estimated using the method described in Chapter 3. The softening systems were assumed to have the same CAPEX as the DOC removal systems of equivalent size. CAPEX, in general, however, can vary widely based on location, manufacturer, site conditions, and other variables. Therefore, the CAPEX values reported here are only general estimates for the purpose of comparison and may not take into account all of the potential capital costs of the system.

4.2.6 Data Quality

The systems evaluated in this study have a groundwater source with low turbidity and are therefore typical of the Floridian peninsula. The results, therefore, are representative of this region and other areas with similar water quality. Furthermore, it may provide insight into other IX applications with similar water characteristics, such as nitrate removal from groundwater. In many regions, high DOC concentrations are not found in groundwater but are found in surface waters with high turbidity. IX systems with influent water sources that have high turbidity may encounter operational issues that must be taken into account in a fair assessment of IX technology. For example, in some instances, high turbidity may require pre-treatment before FBR treatment can be performed, in order to prevent issues of clogging. This additional treatment can incur additional costs and environmental impact that must be assessed on a case by case basis.

Most LCA and LCCA studies of IX systems only take into account evaluation of one system or scenario (Choe et al., 2013; Choe et al., 2015; Dominguez-Ramos et al., 2014; Ras and von Blottnitz, 2012). However, design, installation, and operation of systems can vary significantly. Therefore, it is preferable to study multiple systems to provide a reasonable range of possible conditions, such as conducted in Amini et al. (2015). The data on the CCAE, FBR softening, and CFMR softening systems are based on individual scenarios. Therefore, alternative operating procedures can possibly alter the material and energy usage of these systems, providing better performance of the softening systems. The data included in this study on the DOC removal systems, however, are based on the data collected in Amini et al., (2015) as well as additional assessment performed in Chapter 3. Therefore, the data for these systems provides a reasonable assessment for a typical IX system for removing DOC because the study takes into account multiple systems and uses operational parameters that are reasonable for reducing impacts and costs.

4.3 Results and Discussion

4.3.1 Life Cycle Inventory

The LCI results show the compiled materials, chemicals, energy, and transport required during the operating phase of each of the configuration scenarios evaluated. In order to fully understand the differences between the scenarios, it is necessary to understand the clear differences found between IX systems for softening and those for removing DOC. Furthermore, this research also represents the first LCI and LCA that offers a comparison of these two systems. The LCI of the four individual systems for softening or DOC removal is shown in Table 4.2. The results show that FBR softening systems tend to require approximately 5 times as much salt as FBR systems for removing DOC, while CMFR softening systems require approximately 3.7 times as much salt as CMFR systems for DOC removal over a 20 year time period. This translates into high brine waste production as well, with softening systems possibly generating over 10 times as much brine. This brine, however, is much more diluted because the softening system uses more water for resin rinsing. Furthermore, Amini et al. (2015) noted that in FBR DOC systems it is important to maintain the resin regularly with periodic cleaning. This assessment takes into account a well-maintained FBR DOC system, with resin cleaning every three years. Therefore, if the resin is not as well maintained, the salt usage and brine waste production would be higher, due to the need for more frequent regeneration. FBR systems for softening and DOC removal tend to require similar amounts of resin. However, in CMFR systems, almost 3 times as much resin is required for DOC removal. This is because the MIEX DOC resin tends to break down during usage, requiring continual replenishment of 1-2 gallons of resin per MG of water treated (Amini et al., 2015). The differences in chemical/material requirements causes the softening systems to require 1.5-2.8 times as much transport by barge and 2.8-4.7 times as much transport by truck, measured in ton-kilometers (tkm). Therefore, in general, IX softening systems tend to require more salt, generate more brine, and require more transport than IX DOC systems. However, energy requirements for the systems that remove hardness or DOC are similar.

When comparing FBR softening to CMFR softening systems, the fixed bed systems appear to use less than half as much salt for the regeneration process. The FBR systems produce twice as much brine waste due to using more water volumes during brine rinses and backwashes; however, this brine is more diluted because the mass of salt in the brine is generally the same as the salt usage for each system. This is generally preferable because in most cases the waste brine is sent to the WWTP and more dilution prevents shock loads to the WWTP. The CMFR systems also use approximately 30% more energy than the FBR systems. This is likely due to continuous mixing that is required in the CMFR systems (Amini et al., 2015). Resin usage is also more than 20% higher in the CMFR softening systems. Contrary to the MIEX DOC resin, the MIEX softening resin is not expected to break down significantly. Therefore, this difference likely due to a lower capacity in MIEX softening resin. The higher material requirements of the CMFR systems also lead to more than twice as much barge transport and truck transport requirements compared to FBR systems. It should be noted, however, that the MIEX softening system is a newer technology and is rarely used alone. Therefore, as more experience is gained with the system, additional needs may be recognized, such as a need for periodic resin cleaning.

Furthermore, the disadvantages of the MIEX softening technology noted above may be why the system is not yet widely used. Its design may also contribute to higher material usage of a CCAE system that incorporates it.

Table 4.2: LCI results of the individual softening and DOC removal systems

	FBR SOFT	FBR DOC	CMFR SOFT	CMFR DOC	Units
Salt usage	1,076	218	2,371	647	tons/20 years
Brine waste generated	12,869,022	1,196,913	6,350,561	1,731,971	gal/20 years
Electricity Usage	169,181	167,700	221,699	220,801	kWh/20 years
Chemicals (50% NaOH for FBR, 36% HCl for CMFR)	-	4,550	-	32,558	kg/20 years
Boat Transport	725,152	253,265	1,513,477	978,710	tkm/20 years
Truck Transport	162,681	34,667	357,315	129,485	tkm/20 years
Resin Usage	8,903	8,903	11,080	32,966	kg/ 20 years

Among the six scenarios evaluated that include both DOC removal and softening, significant differences can also be seen. The LCI results of these scenarios are shown in Table 4.3. In regards to the LCI it was hypothesized that the CCAE system would have lower salt usage and brine waste production than conventionally separate IX systems. The results show that the theoretical CCAE system, which is based in a CMFR design, has lower salt usage and brine waste than two separate CMFR systems. This is due to CCAE's ability to reuse the same brine for regenerating both types of resin, utilizing both the cation and anion of the salt. Furthermore, the theoretical CCAE system is preferable to the FBR DOC system with CMFR softening. This is mainly due to the high salt requirements of the CMFR softening system. However, the two scenarios which incorporate FBR softening use far less salt than the theoretical CCAE system. This is likely due to the advantages of the FBR softening over CMFR softening, noted above. The theoretical system also generates less brine waste than all of the other scenarios; however, as noted above, the waste brine from the FBR systems are much more diluted. Therefore, the brine waste generated from the FBR systems are generally preferable because they add less overall total dissolved solids to the WWTP. In terms of energy usage, the CMFR systems, including CCAE, generally tend to use more energy than the FBR systems. Barge transport and truck transport for the theoretical CCAE system are less than for scenarios that use CMFR softening, which is mainly due to the lower amount of salt required; however, the CCAE system requires more transport than the scenarios that use FBR softening.

The results for the actual CCAE system are based on the first treatment plant that is currently utilizing the technology. In comparison to the theoretical CCAE system, the real system requires more salt, generates more brine waste, and requires more transport. Furthermore, the real CCAE system requires more materials, chemicals, and transport than all of the other scenarios for most of the impact contributors. The higher salt usage of the real CCAE system is because currently the operators only use fresh brine for regeneration, even though CCAE has the potential to reuse the same brine for both cation and anion regeneration. This is likely due to concern about possible precipitation, which could complicate the regeneration process. Furthermore, the CCAE system appears to use more salt than even two separate CMFR systems for DOC removal and softening. This is likely due solely to overuse of salt by the operators. It is common to over-treat or overuse chemicals to ensure the system does not fail because operators are generally responsible for the successful operation of the plant and avoiding process failure. Therefore, economic and environmental performance may often be sacrificed for technical performance. The actual CCAE system also generates more brine waste than the other scenarios. This is likely due to the same reasons. Operators may choose to provide additional rinsing and dilution to ensure the system does not fail, although such excess water usage may not be necessary. Due to these differences, the actual CCAE system requires more barge and truck transport than any of the alternative scenarios.

Electricity usage in the CCAE system is similar to the combined CMFR systems, but saves slightly due to decreased energy requirements for mixing because only one reactor is required. In terms of resin, the actual CCAE system, which uses a MIEX resin, consumes less resin than other systems with MIEX DOC resin but more than FBR systems. This is because the MIEX DOC resins break down over time whereas the conventional resins used in FBR reactors do not (Amini et al., 2015). However, the CCAE system implements pump mixing instead of mixing by impellers, used by many of the currently installed CMFR systems. The pump mixing introduces less shear forces on the resin, causing it to deteriorate at half the rate of when impeller mixing is used. This is not an inherent benefit to the CCAE technology but represents an advancement in IX CMFR design. In regards to softening resin, however, the CCAE systems use more than any of the other scenarios. This is because more MIEX softening resin tends to be required as compared to the conventional FBR softening resin. Furthermore, implementing cation and anion exchange resins in the same reactor potentially reduces overall exchange efficiency, requiring more resin. The main advantage the actual CCAE system holds is that it appears to require far less chemicals than the other scenarios; however, as experience is gained with the system, the need for more chemical addition may be recognized in the future.

A possible modification that can improve the performance of CCAE is to use it in a FBR-based design. As shown above, the FBR systems appear to require less salt, use less electricity, use less resin, and require less transport overall compared to CMFR systems. Therefore, implementing CCAE in a FBR-based design instead of a CMFR-based design may provide far more environmental and economic benefits. However, it is important to ensure that proper testing and piloting of such systems is performed to prevent potential issues with precipitation and clogging that can occur with multiple resin types in a fixed bed.

Table 4.3: Life cycle inventory results for six scenarios

	CCAE (Theoret.)	CCAE (Actual)	FBR DOC + FBR SOFT	FBR DOC + CMFR SOFT	CMFR DOC + FBR SOFT	CMFR DOC + CMFR SOFT	Units
Salt usage	2,371	3,629	1,293	2,589	1,722	3,018	tons/20 years
Brine waste generated	6,350,561	37,960,000	14,065,936	7,547,474	14,600,994	8,082,532	gal/20 years
Electricity Usage	360,846	360,846	336,881	389,399	389,982	442,500	kWh/20 years
Chemicals (50% NaOH)	-	-	4,550	4,550	-	-	kg/20 years
Chemicals (36% HCl)	1,070	1,070	-	-	32,558	32,558	kg/20 years
Boat Transport	1,966,173	2,657,920	978,418	1,766,742	1,703,862	2,492,187	tkm
Truck Transport	361,068	549,726	197,349	391,982	292,166	486,800	tkm
DOC Resin	22,023	22,023	8,903	8,903	32,966	32,966	kg DOC resin/ 20 years
Softening Resin	13,009	13,009	8,903	11,080	8,903	11,080	kg SOFT resin/ 20 years

4.3.2 Impact Assessment

The life cycle impact assessment (LCIA) was calculated using the inventory results for each of the individual IX systems as well as the six combined IX system scenarios. The environmental impacts of the four individual systems are shown in Figure 4.2, showing the contribution of each component of the LCI to the overall impact. The order of systems from highest to lowest environmental impact is: CMFR Softening > CMFR DOC removal > FBR Softening > FBR DOC Removal. The four inventory items that contribute most to the environmental impact are salt usage, brine waste treatment, resin usage, and electricity usage. In softening systems, the highest impact contributor is salt usage. Softening systems also tend to have much higher impact due to salt usage then the DOC removal systems. Furthermore, the impact due to brine waste treatment at the WWTP is high in softening systems. The highest impact contributor for the CMFR DOC removal system is resin usage, which is due to breakdown of the MIEX DOC resin, as described above. The other systems use a relatively similar amount of resin. The systems also have similar impacts from electricity use, but CMFR systems have slightly higher impact, which is consistent with Amini et al. (2015). The FBR DOC systems have the lowest impact overall, and the impact is approximately evenly divided among resin, electricity, and salt usage. The FBR systems in general also tend to have lower impact than their CMFR counterparts. This is also consistent with results in Amini et al. (2015), who found that FBR DOC removal systems can have lower environmental impacts than CMFR DOC removal systems, when the resin is regularly cleaned.

The environmental impact results of the six combined IX scenarios reflect the strengths and weaknesses of the individual IX systems, as shown in Figure 4.3. For example, the systems that include CMFR softening tend to have higher environmental impacts. This includes the CCAE system, which is a CMFR design. The high impact is due largely to high salt usage and brine waste treatment.

The theoretical CCAE has lower impact than CMFR softening with CMFR DOC removal. This is due to the reduction in salt usage and brine waste production noted in the LCI.

However, the actual CCAE system has much higher impact because it does not reap the benefits of brine reuse during regeneration, as discussed in the LCI. Overall, utilizing an FBR

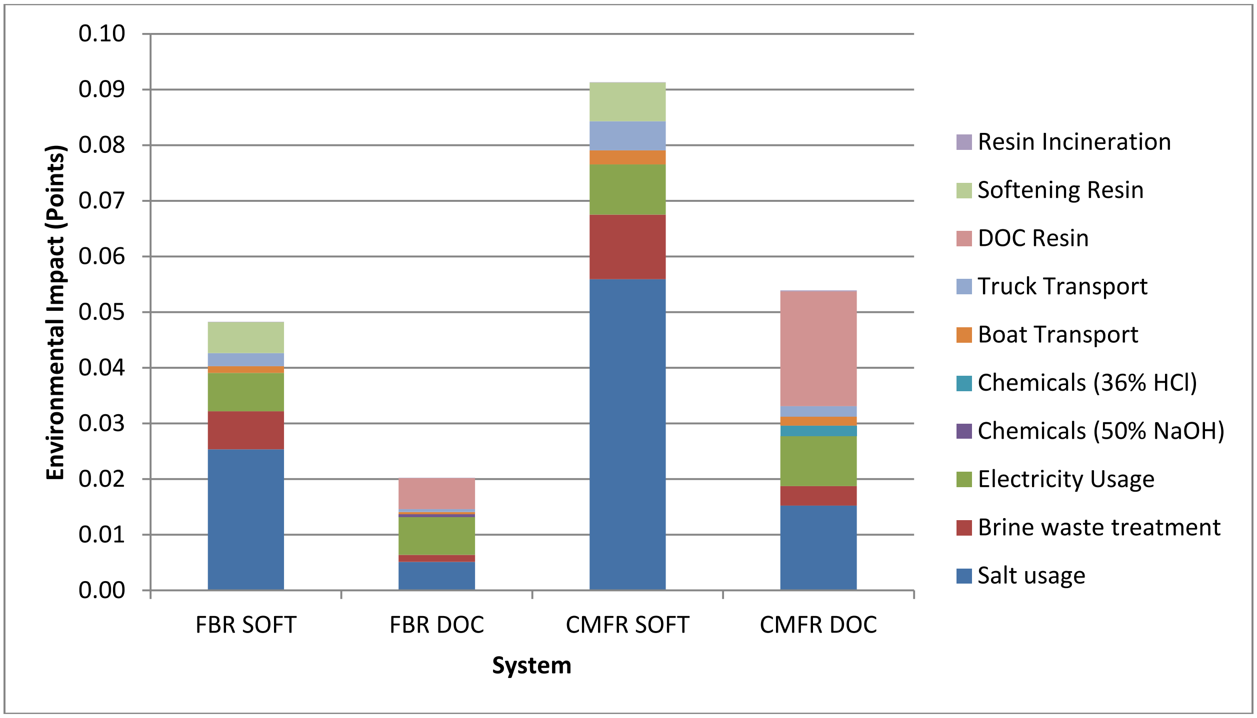


Figure 4.2: Environmental impact of separate IX systems

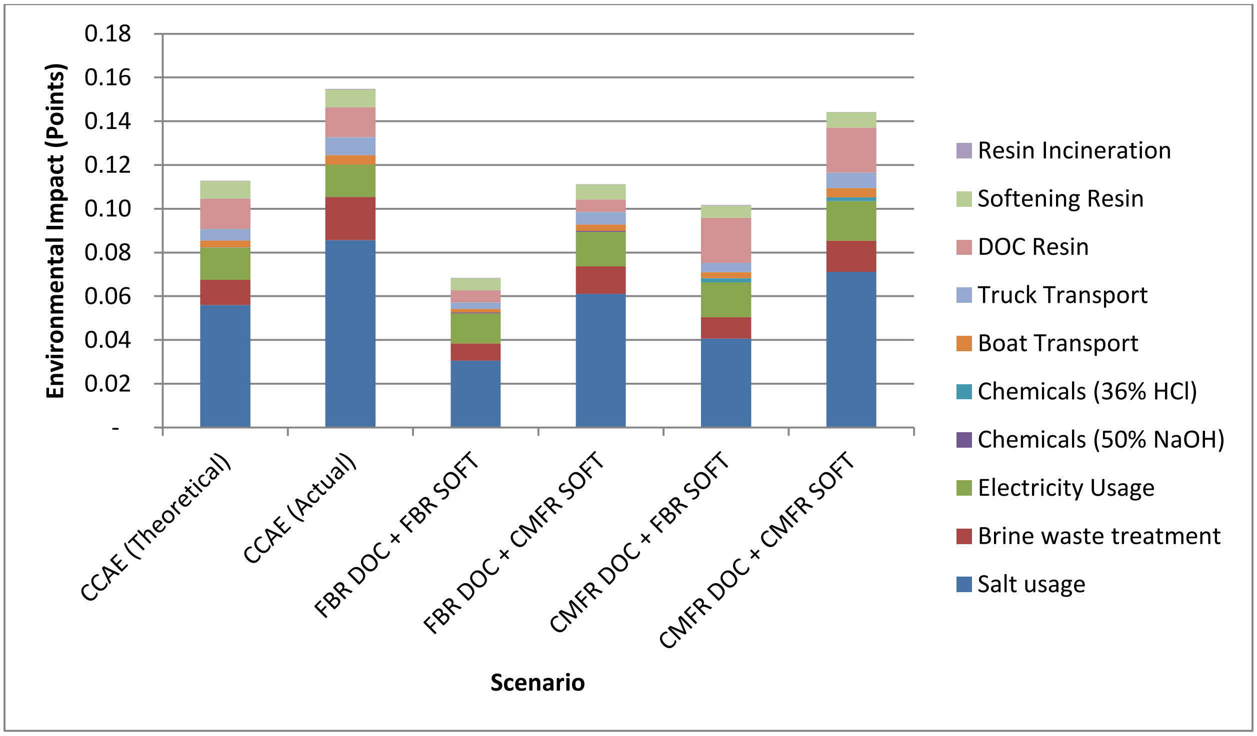


Figure 4.3: Environmental impact of six combined IX scenarios

configuration provides the least environmental impact and far outweighs the benefits of using CCAE with CMFR systems. Consistent with the LCI results, implementation of CCAE technology with FBR systems could potentially provide the most benefit in terms of environmental impact.

4.3.3 Life Cycle Cost Analysis

The operation cost for the individual systems and the combined system scenarios were calculated using the inventory results. These costs represent best estimates and may, of course, vary by region, supplier, and material selection. The operation costs for the four individual IX systems follow similar patterns to the LCI and LCIA results, as shown in Figure 4.4. Overall, the softening systems have higher costs than the DOC removal systems and the CMFR systems have higher costs than FBR systems. The CMFR softening system incurs the highest operation cost of approximately $425,000 over a 20 year time period while the FBR DOC system has the lowest cost of approximately $150,000.

The operation costs of the combined scenarios follow similar patterns as the LCIA results; however, the salt takes on less importance because it is inexpensive, whereas usage of costly resin takes on more importance. These results are shown in Figure 4.5 Therefore, the systems that incorporate CMFR DOC removal will tend to have high costs due to the high resin usage. This also includes the CCAE system, but, as noted above, the CCAE system requires less resin replenishment due to using pump mixing. Nevertheless, the scenarios that include CMFR softening tend to have higher costs due to the high salt usage. The brine treatment cost averages approximately $95,000 over the 20 year time period. These costs, however, are not incurred to the WTP but are costs to the WWTP due to higher aeration and carbon source requirements for

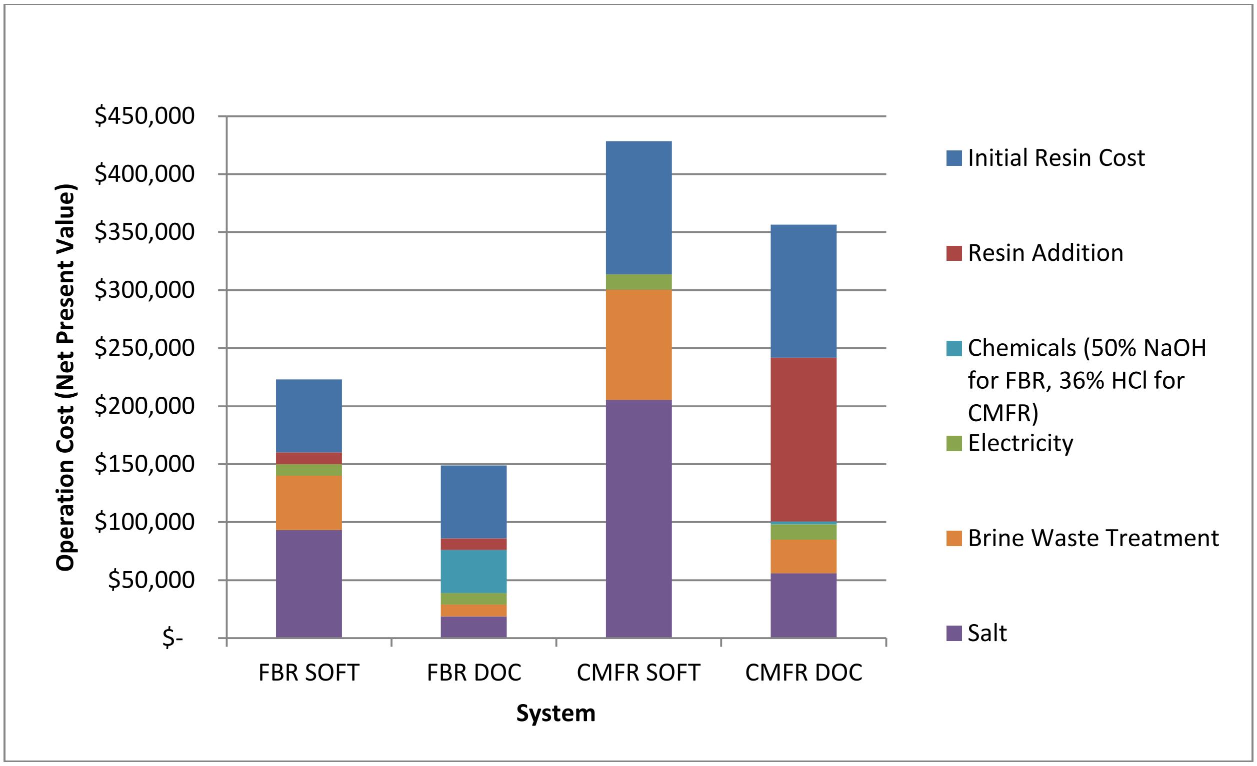


Figure 4.4: Operation cost of separate IX systems in net present value for 20 year time period

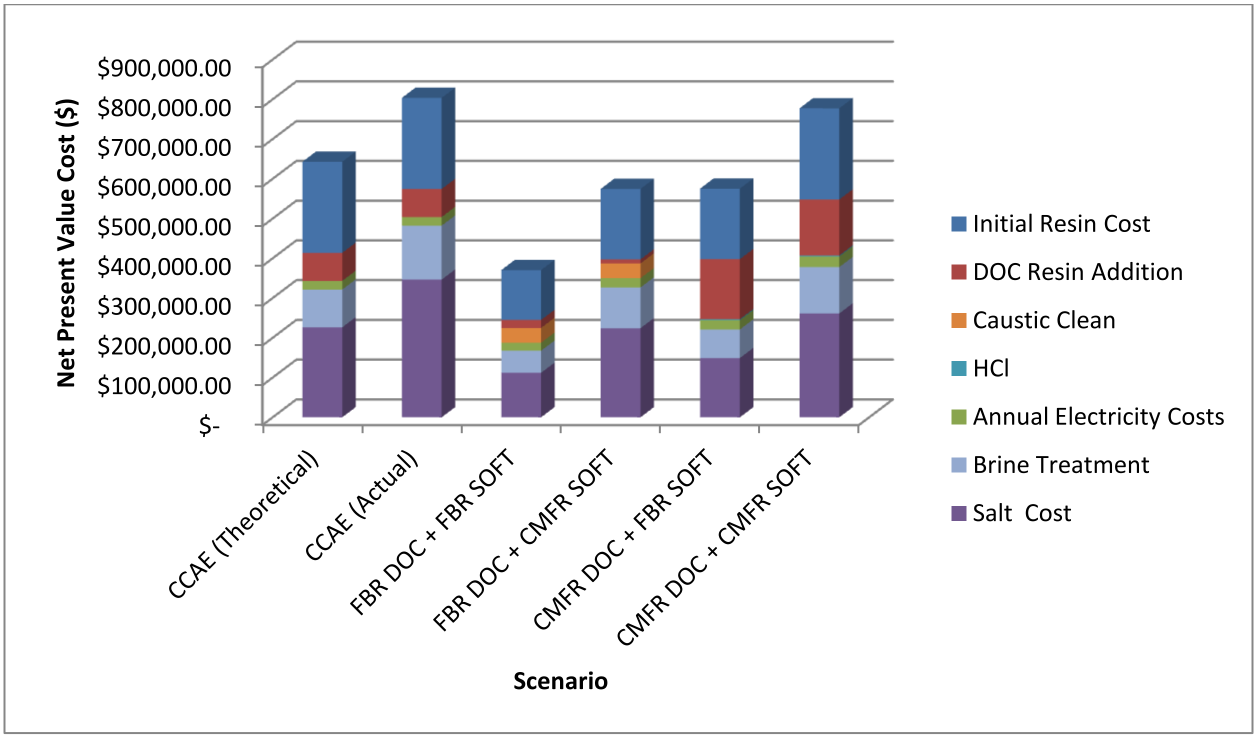


Figure 4.5: Lifetime operation cost of the six scenarios

activated sludge treatment, nitrification, and denitrification. However, in many cases the WTP and WWTP are owned by the same utility and cost savings from both are desirable.

The capital costs for an individual FBR or CMFR system are estimated at about $600,000 for each system. However, these costs can vary significantly from installation to installation, depending on the system requirements. A typical combined system is therefore approximately $1.2 million. However, the lifetime of the FBR systems was approximated by manufacturers at 30 years whereas the CMFR system life was estimated at 20 years. Therefore, the FBR softening with FBR DOC removal has the lowest capital cost of approximately $800,000 for a 20 year period.

The estimated capital cost, total operation cost, and life cycle cost of each of the four combined scenarios are shown in Table 4.4. Because there is only one known installation of CCAE, it is more difficult to approximate the costs. However, it may be assumed that it has a slightly lower capital cost than the CMFR DOC removal and CMFR softening scenario, due to the need for less reactors and equipment. If this is the case, the CCAE system has a life cycle cost that is slightly lower than the CMFR DOC removal and CMFR softening scenario. Overall, the FBR DOC removal and FBR softening scenario provide approximately $650,000 in savings over a 20 year time period compared to the CCAE system. Utilizing CCAE technology in a fixed bed design could possibly reduce cost, due to reduced infrastructure requirements and salt/brine

Table 4.4: Estimated capital, operation, and total costs in NPV for 20 year time period

	Combined (Theoretical)	Combined (Actual)	FBR DOC + FBR SOFT	FBR DOC + CMFR SOFT	CMFR DOC + FBR SOFT	CMFR DOC + CMFR SOFT
Capital Cost ($)	1,100,000	1,100,000	797,439	996,799	996,799	1,196,158
Operation Cost ($)	643,023	667,962	314,976	472,114	503,551	660,689
Total Cost ($)	1,743,023	1,767,962	1,112,415	1,468,913	1,500,350	1,856,847

reduction. However, there must be sufficient testing of such systems to ensure that fouling or clogging do not make CCAE technology impractical from a technical standpoint for implementation in an FBR configuration.

4.4 Conclusion

IX softening systems tend to require more salt, generate more brine, and require more transport than IX DOC systems. This translates into lower environmental impacts and operation costs being incurred by DOC removal compared to equivalent softening systems. Furthermore, FBR systems tend to generally require less salt, energy, and resin than CMFR systems. Although FBR systems generate more brine waste by volume than CMFR systems, the brine is more diluted, which is preferable in preventing shock loads when the waste brine is discharged to the wastewater treatment plant. Moreover, FBR systems have lower impacts and costs than equivalent CMFR systems. Due to the longer lifetime of FBR systems, the capital cost is also effectively lower than CMFR systems.

Theoretically, CCAE systems can provide advantages to the combination of two separate IX systems. In this case, the theoretical CCAE system, which is based in a CMFR design, was found to have lower impacts and costs than a combination of CMFR systems. However, the system must be properly designed in actual installations to take account of its potential advantages which can reduce salt requirements, brine waste generation, and infrastructure requirements. Operators must also be trained to appropriately implement brine reuse in CCAE systems to reduce environmental impacts and costs from salt usage and brine waste treatment. Moreover, utilizing CCAE with a reactor design that has lower overall impacts and costs will further maximize its benefit.

4.5 References

Amini, A., Kim, Y., Zhang, J., Boyer, T., Zhang, Q. (2015) Environmental and Economic Sustainability of Ion Exchange Drinking Water Treatment for Organics Removal. Journal of Cleaner Production. http://dx.doi.org/10.1016/j.jclepro.2015.05.056

Apell, J., & Boyer, T. (2010). Combined ion exchange treatment for removal of dissolved organic matter and hardness. Water Research, 2419-2430.

Bare, J.C., Norris, G.A., Pennington, D.W., McKone, T., 2003. TRACI - the tool for the reduction and assessment of chemical and other environmental impacts. J. Ind. Ecol. 6, 49-78.

Bare, J., Gloria, T., Norris, G., (2006). Development of the method and U.S. normalization database for life cycle impact assessment and sustainability metrics. Environ. Sci. Technol. 40, 5108-5115.

Comstock, S., & Boyer, T. (2014). Combined magnetic ion exchange and cation exchange for removal of DOC and hardness. Chemical Engineering Journal, 241, 366-375.

Dominguez-Ramos, A., Chavan, K., García, V., Jimeno, G., Albo, J., Marathe, K. V., Yadav, G. D., Irabien, A., (2014). Arsenic Removal from Natural Waters by Adsorption or Ion Exchange: An Environmental Sustainability Assessment. Industrial and Engineering Chemistry Research 53, 18920-18927.

Fu, L., Liu, F., Ma, Y., Tao, X., Ling, C., Li, A., . . . Li, Y. (2015). High-efficient technique to simultaneous removal of Cu(II), Ni(II) and tannic acid with magnetic resins: Complex mechanism behind integrative application. Chemical Engineering Journal, 263, 83-91.

Indarawis, K., & Boyer, T. (2013). Superposition of anion and cation exchange for removal of natural water ions. Separation and Purification Technology, 118, 112-119.

ISO, 2006a. Environmental ManagementdLife Cycle Assessment: Principles and Framework. ISO14040. International Standard Organisation, Geneva.

ISO, 2006b. Environmental ManagementdLife Cycle Assessment: Requirements and Guidelines. ISO14044. International Standard Organisation, Geneva.

Maul, G., Kim, Y., Amini, A., Zhang, Q., Boyer, T., (2014). Efficiency and Life Cycle Environmental Impacts of Ion-exchange Regeneration Using Sodium, Potassium, Chloride, and Bicarbonate Salts. Chemical Engineering Journal. 254, 198-209.

Panswad, T., Anan, C., (1999). Impact of High Chloride Wastewater on an Anaerobic/anoxic/aerobic process with and without Inoculation of Chloride Acclimated Seeds. Water Research. 33, 1165-1172.

Ras, C., von Blottnitz, H., (2012). A comparative life cycle assessment of process water treatment technologies at the Secunda industrial complex, South Africa. Water SA. 38, 549-554.

United States Environmental Protection Agency (USEPA). (2013). 2013 National Public Water Systems Compliance Report (EPA DOCUMENT 305R15001).Washington, DC: Office of Enforcement and Compliance Assurance (2201A).

4.6 Supporting Information

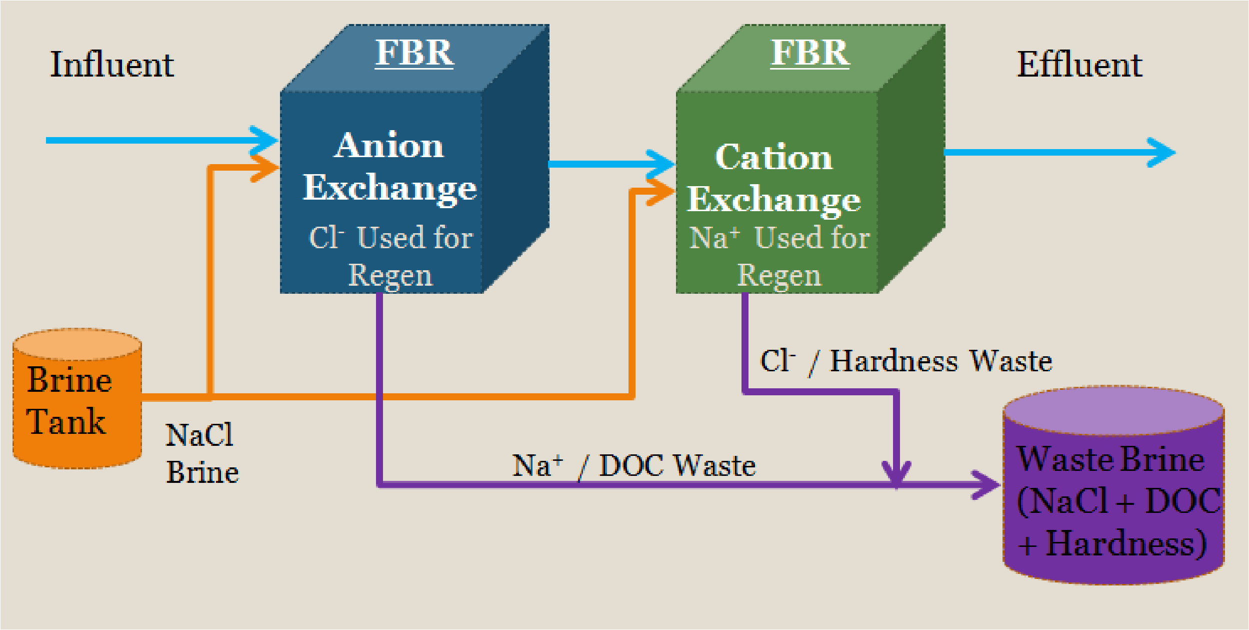


Figure 4.6: System configuration using a FBR for both anion and cation exchange

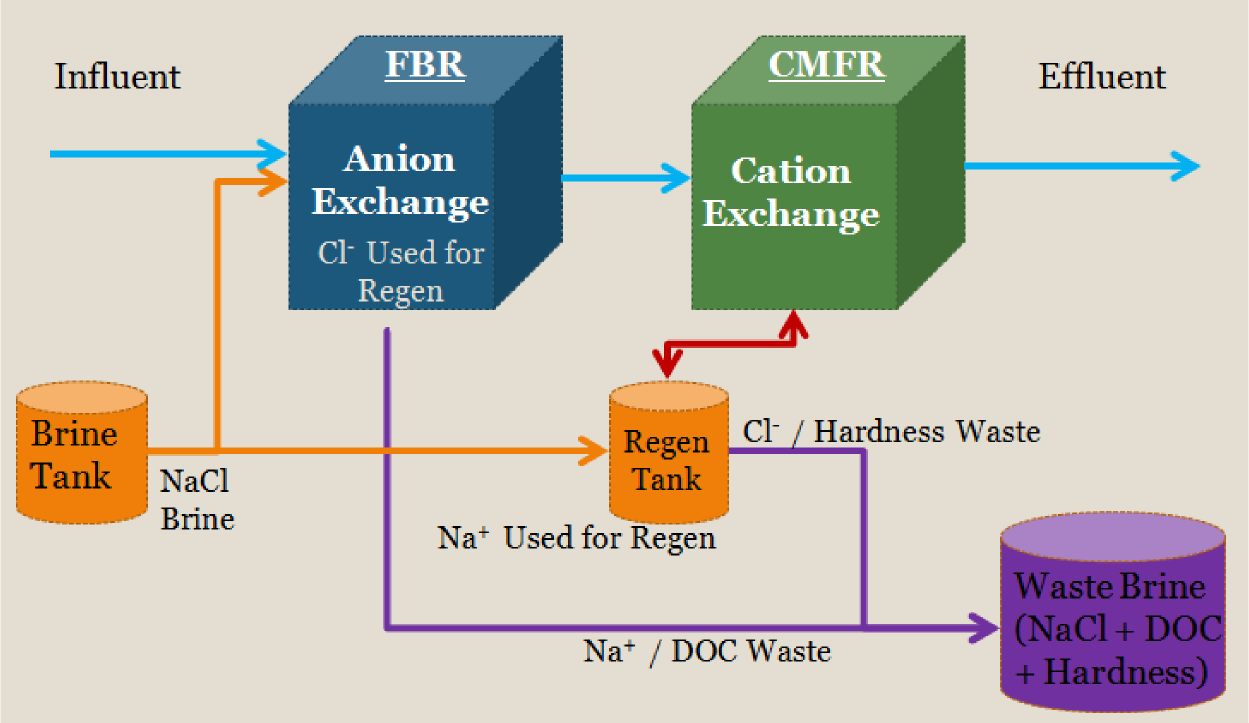


Figure 4.7: System configuration using a FBR for anion exchange and a CMFR for cation exchange

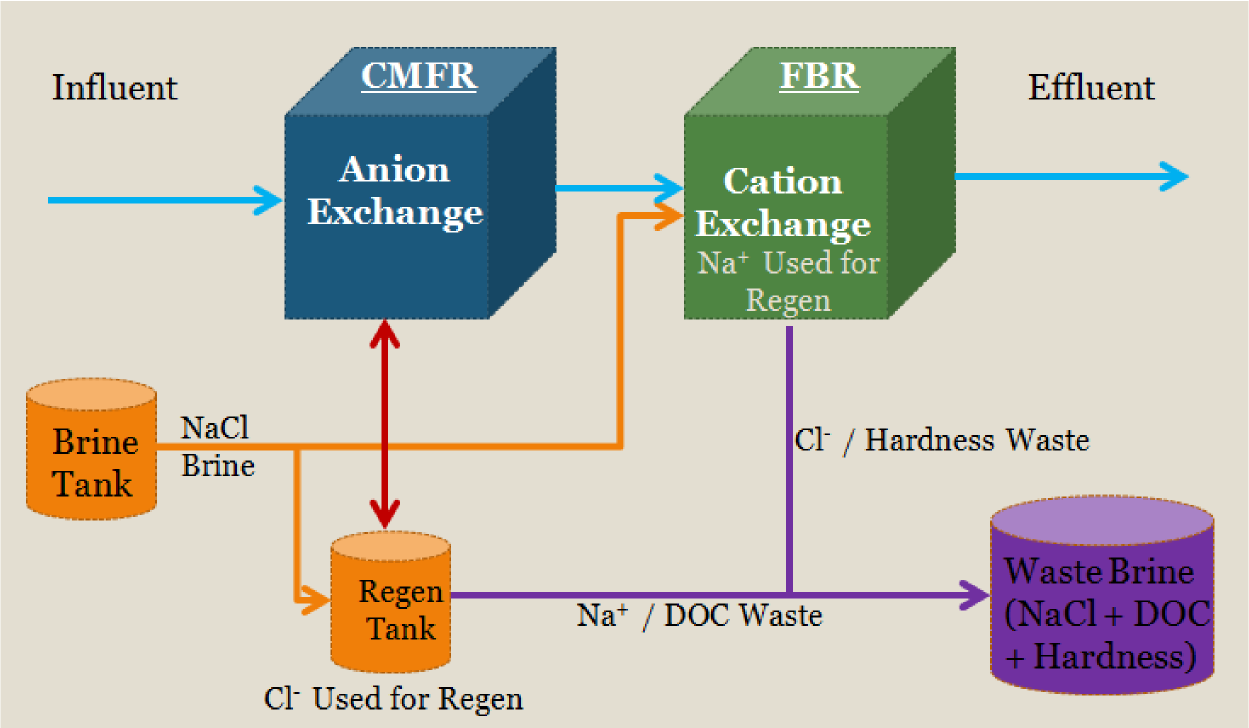


Figure 4.8: System configuration using a CMFR for anion exchange and a FBR for cation exchange

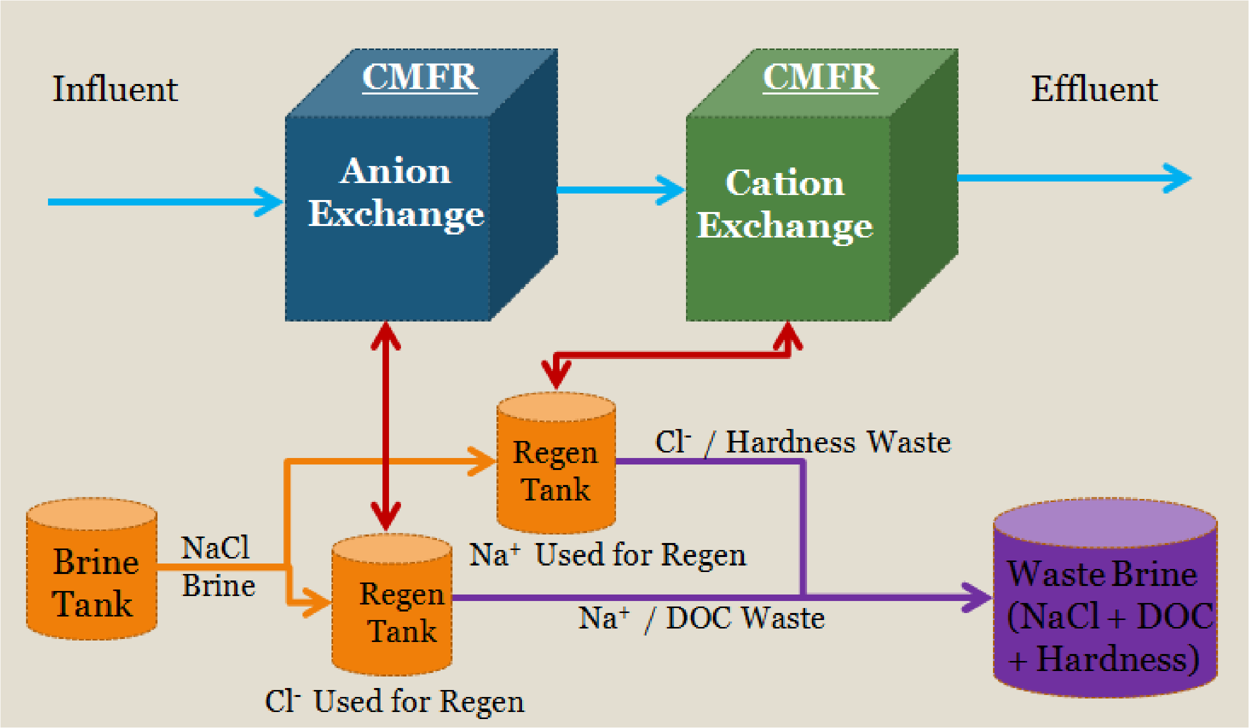


Figure 4.9: System configuration using a CMFR for both anion and cation exchange

Chapter 5: Research Dissemination to Water Professionals (Task 4)

There has long been recognized a disconnect between science and practice which prevents the application of research results (Bero et al., 1998; Buckley et al., 1998; Bansal et al., 2012; Langrall, 2014). Research results often do not reach the community of interest that they are applicable to and academic methods, language, and tools are not accessible to practitioners due to differences in training, education level, and access to literature and resources. Furthermore, there is often a gap between that which is applicable (what is relevant) and that which is actionable (how to implement it in the world) (Argyris and Schon, 1974).

Therefore, engaging with the practitioner community requires making scientific knowledge actionable. Furthermore, methods often fail when the community of interest is not included in the decision making process (Arches, 1999). Therefore, there must be a collaborative relationship between the scientists and practitioners in order to successfully bridge the research/practice gap (McCown, 2001). While engaging with stakeholders remains an area of learning, one of the basic methods that is commonly used is holding meetings with stakeholders and using surveys to generate stakeholder input. Science has also developed to take into account a more holistic approach, not only modeling basic process (e.g. physical, chemical, physiological, etc.) but whole processes, which allows models to identify optimal designs and outcomes. Development of such models through computer-based programs has been another method to allow the scientific community to intervene in the community of practice (McCown, 2001). However, such models are often complex and difficult to use, which makes them not directly accessible to practitioners. A user-friendly decision tool can make such models accessible to the drinking water community.

The primary goal of Task 4 is to disseminate results of research among stakeholders and develop a simplified tool for evaluating and comparing sustainability of IX system designs that can be used by the drinking water community and takes into account their feedback. This can be divided into several specific objectives. The first objective is to hold meetings with treatment plants that directly participated in the studies carried out, particularly the IX treatment plants in Florida, and to share with them the results of the studies. The second objective involves developing a user-friendly tool that can be used to evaluate and compare the environmental impacts and costs are various IX designs. This tool can be distributed among stakeholders and make the research findings accessible to the community of interest. In regards to the third objective, several researchers have been developing a sustainability assessment framework (SAF) with semi-quantitative matrix that allows for assessment of water treatment plants, including IX plants, from the perspective of various sustainability dimensions and criteria. The purpose of objective 3 is to include stakeholder feedback in the development of the SAF rating mechanisms. This is achieved through the use of surveys to develop an appropriate weighting scheme for the sustainability criteria. These objectives provide a channel for allowing the research in this dissertation to better reach the community of interest. Furthermore, they allow for development of tools that are actionable in the field and they take into the stakeholder feedback in the development of those tools. The three objectives, as well as their results, are described in detail in the sections that follow.

5.1 Objective 1: Meetings with IX Plants

Throughout the Fall and Spring of 2016, contact was made with each of the plants that participated in the studies carried out in Tasks 1-3 to hold meetings where the author shared the results of our studies and discussed any questions that they employees of the treatment plant had. Six of the eight plants that participated in the previous studies agreed to host a meeting and, among these facilities, over 22 individuals participated, including superintendants, operators, and other administrators.

With certain plants there was discussion of possible actionable changes that the treatment plant could make to reduce their costs and environmental impacts. For example, there was a discussion with staff from two of the treatment plants on how they could implement regular resin cleaning procedures, which they currently lack. They were shown cost and environmental impact comparisons to other treatment plants that have such procedures in place and they were provided contact information of the other plants so that they could seek assistance or ask advice from them. Furthermore, with the treatment plant that was already implementing regular resin treatment, the benefit of the process was discussed with them and they were encouraged to continue the practice.

The verbal feedback regarding these meetings was very positive and employees of the treatment plants expressed appreciation for having the results shared with them. The attendees expressed that often when studies are carried out on their facilities or on technology that is relevant to them, they never see the results of the research and therefore do not have the opportunity to learn from the experience. They also seemed to appreciate the opportunity to interact with someone from academia and discuss issues that they have experienced.

5.2 Objective 2: Development of a User-Friendly Tool

The objectives of Task 2 led to the development of a model that integrates process models with LCA and LCCA. This allows for the assessment of a various design scenarios, where the user can specify particular design characteristics of the IX system, such as the reactor type and hydraulic retention time (HRT), and estimate the environmental impacts and costs of that system.

This model, however, is limited in its accessibility due to its difficulty of use, which requires expertise in computer science. Furthermore, it requires ownership of propriety software, particularly Matlab, which can be costly. These challenges make the model inaccessible to much of the drinking water community and limit the impact of the research. Development of a tool with a user-friendly interface that does not require specific coding expertise and does not require expensive software allows for use of the model by the drinking water community.

Several options were explored for the creation of the tool, including web-based or excel based applications. However, these options required complex transfer of the code’s capabilities into an alternative software. Therefore, the method that was chosen for creating the tool is Matlab’s App Designer, which is fully compatible with the original code that was created in Matlab. The tool is able to access and run the original code while providing a number of additional features. Furthermore, it has the ability to be utilized by individuals who do not own Matlab software. Therefore, the tool is a standalone application that requires no other software for its use.

The tool has been named the Sustainability of Ion Exchange Simulator (the SION Simulator). SION is currently designed to provide functionality for the code’s main functions, which include assessment of fixed bed reactor (FBR) and completely mixed flow reactor

(CMFR) designs of IX systems that remove dissolved organic carbon (DOC). However, if increased functionality is added to the original code, such as the ability to assess IX systems that remove other contaminants, the tool can be modified to include the new capabilities with relative ease by individuals who have the original files and reasonable Matlab expertise.

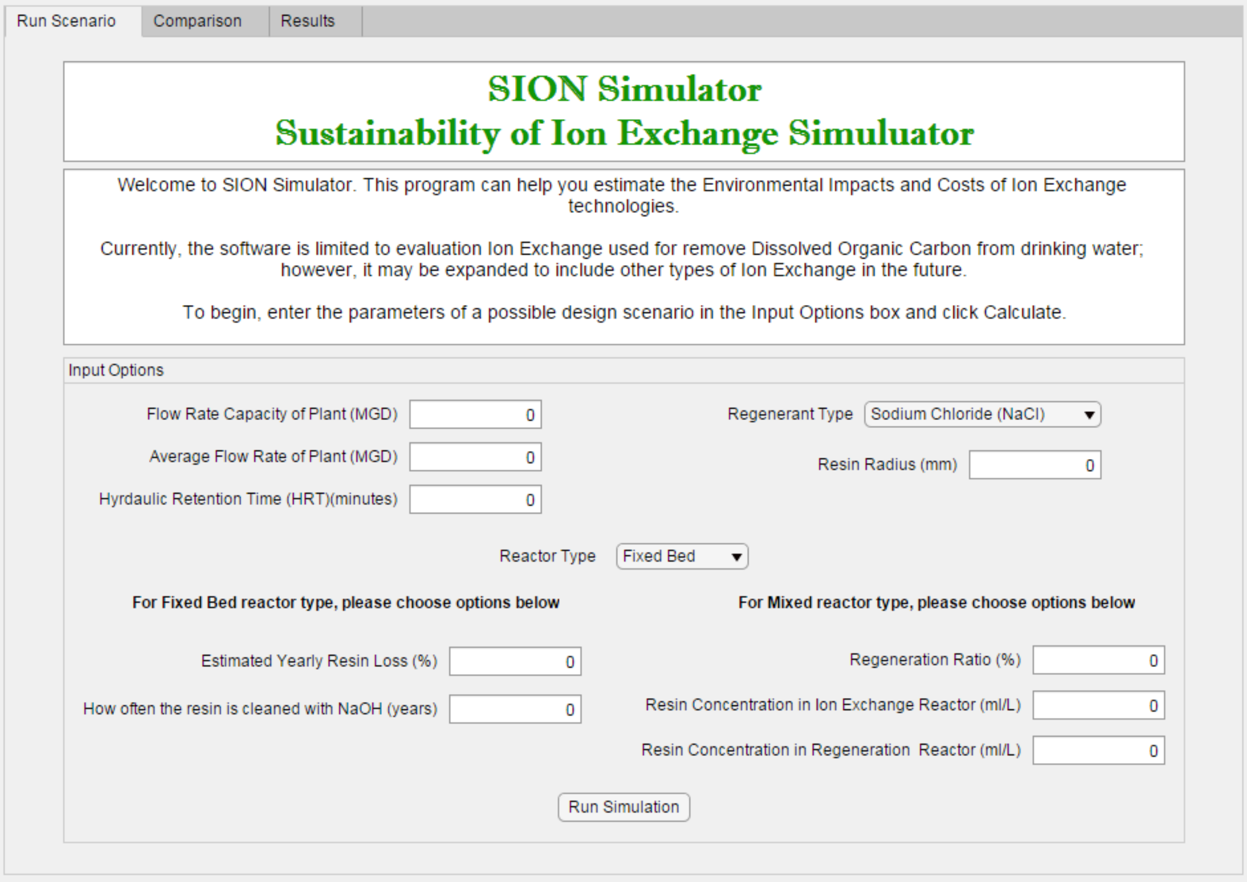
SION includes features such as the ability to evaluate a single scenario or compare two scenarios. It provides a user-friendly interface that is accessible for individuals who have little computer experience. Furthermore, SION provides automatic generation of figures and graphs so that the user can easily interpret the results.

SION includes a continually updating database of results of various scenarios. When a given scenario is run by the user, SION checks the database to see if that scenario has been run previously. If the scenario is already in the database, then SION will draw the results from the database immediately and display the appropriate outputs. If the scenario has not been run before, then SION will access the original code created in Task 2 to run the given scenario and will then add the results to the database so that it is available in the future. In some cases, the code can take approximately 30-45 minutes to run a single scenario, but with most scenarios the code will take a few seconds to a few minutes of time. Therefore, the updating database saves the user valuable time because it does not have to rerun a particular scenario every time the SION software is used.

SION’s inputs includes eleven design options, including reactor type, resin radius, regenerant type, hydraulic retention time (HRT), flow rate capacity of the system, and average flow rate of the system. Some of the design options are particular to FBR or CMFR systems, such as resin attrition rate and how often the resin is cleaned for FBR systems. For CMFR systems, the user must also specify the regeneration ratio, resin concentration in the main contactor, and resin concentration in the regeneration reactor.

SION's outputs include graphs that display the estimated life cycle inventory (LCI) of the operation phase of the IX system, which shows the energy and materials used during the systems operation. Furthermore, figures are generated that show the estimated environmental impact of the system scenario and show how much of that impact is attributable to different impact contributors (elements of the LCI). For example, the user can view how much of the impacts are due to salt production, electricity use, and so on. This is achieved through stacked and clustered column graphs. The impacts displayed include the ten impact categories assessed in the TRACI 2.0 method, which was developed by the United States Environmental Protection Agency (EPA) and is suited for North America. Figures are also created that display various aspects of the costs, including the estimated construction costs as well as the net present value (NPV) of the operation costs, with a breakdown of how much of the operation cost is attributable to different elements of the LCI. It also displays the NPV of the lifetime systems costs (combines construction and operation), and the NPV of the lifetime system costs that is normalized by the quantity of water treated and quality of water (a functional unit that measures how much of the target species is removed through treatment, as discussed in Chapter 2). Each of these figures can be generated for evaluation of a single scenario as well as for comparison of two scenarios. A screenshot of SION's main screen which is used for running a single scenario is shown in Figure 5.1. This shows how the software interface is simple to use, making it accessible to users for various levels of computer literacy and allowing for users to easily enter parameters and calculate a result. Figure 5.2 shows a screenshot of the SION software tab that allows for comparison of two design scenarios. Once again, it follows a simple and user-friendly format.

The current version of SION includes much of the functionality that would be needed by most users. However, the software is also relatively easy to modify so that new functions can be added in the future. Therefore, as the software is used, feedback that is received can be implemented to improve the software.



SION Simulator
Sustainability of Ion Exchange Simuluator

Welcome to SION Simulator. This program can help you estimate the Environmental Impacts and Costs of Ion Exchange technologies.

Currently, the software is limited to evaluation Ion Exchange used for remove Dissolved Organic Carbon from drinking water; however, it may be expanded to include other types of Ion Exchange in the future.

To begin, enter the parameters of a possible design scenario in the Input Options box and click Calculate.

Flow Rate Capacity of Plant (MGD) 0
Average Flow Rate of Plant (MGD) 0
Hyrdaulic Retention Time (HRT)(minutes) 0
Regenerant Type Sodium Chloride (NaCl)
Resin Radius (mm) 0
Reactor Type Fixed Bed

For Fixed Bed reactor type, please choose options below

Estimated Yearly Resin Loss (%) 0
How often the resin is cleaned with NaOH (years) 0

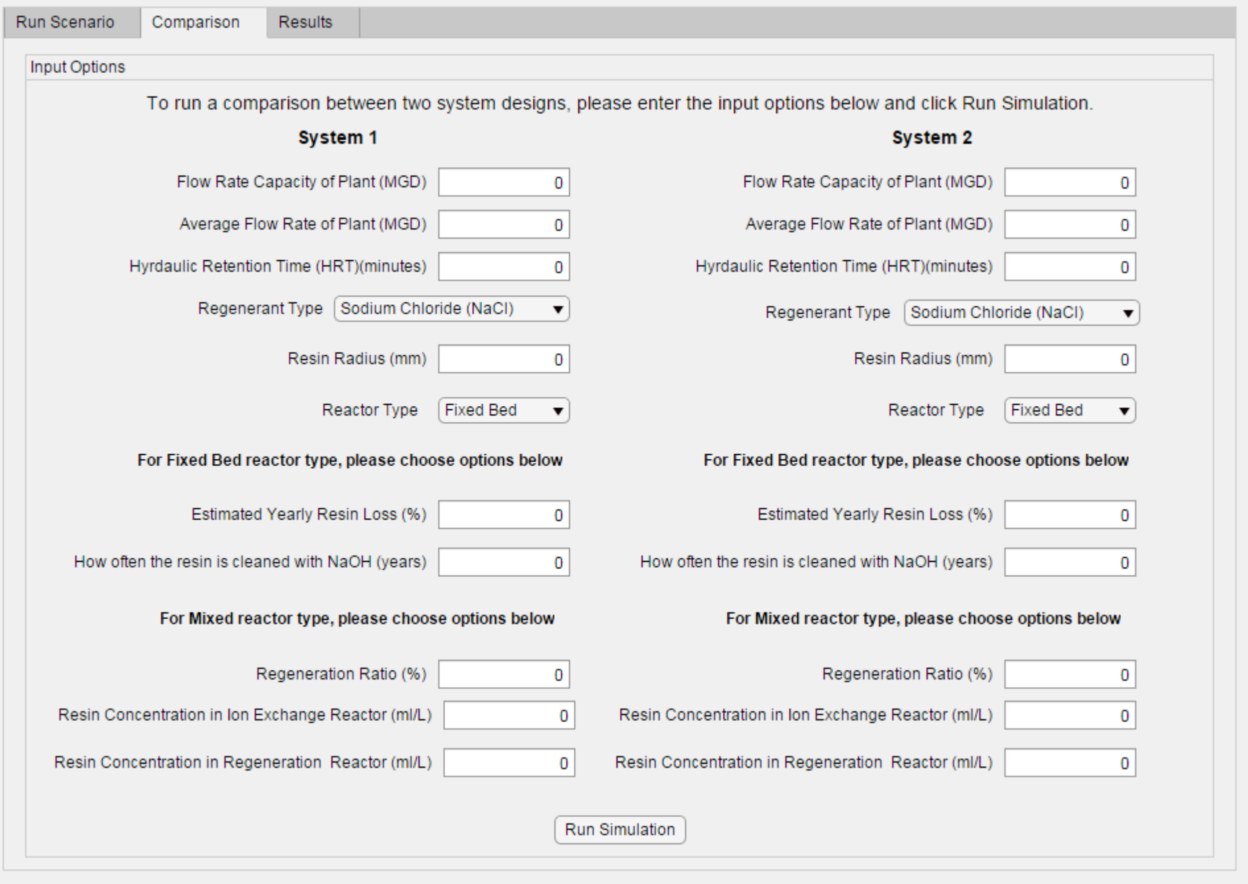
For Mixed reactor type, please choose options below

Regeneration Ratio (%) 0
Resin Concentration in Ion Exchange Reactor (ml/L) 0
Resin Concentration in Regeneration Reactor (ml/L) 0

Figure 5.1: Screen capture of the main page interface of SION simulator, which introduces the tool and allow for running a single scenario

Currently, SION is being conceived of as a free tool for the drinking water community to utilize. However, the design of the software is as a black box and does not allow for access or modification of the code. Currently, it is conceived that individuals who will have access to the code and the ability to modify SION will be limited to researchers collaborating on relevant projects at the University of South Florida. In the future, consideration can be made for making the program open source or improving it further to make it a commercially viable product.

SION therefore provides a simple and easy to use software tool that allow for the research conducted in Tasks 1 and 2 to better reach the community of water professionals. It helps bridge the gap between research and practice, allowing the research to have greater impact while making it directly accessible to the community of practice.



To run a comparison between two system designs, please enter the input options below and click Run Simulation.

System 1		System 2	
Flow Rate Capacity of Plant (MGD)	0	Flow Rate Capacity of Plant (MGD)	0
Average Flow Rate of Plant (MGD)	0	Average Flow Rate of Plant (MGD)	0
Hyrdaulic Retention Time (HRT)(minutes)	0	Hyrdaulic Retention Time (HRT)(minutes)	0
Regenerant Type	Sodium Chloride (NaCl)	Regenerant Type	Sodium Chloride (NaCl)
Resin Radius (mm)	0	Resin Radius (mm)	0
Reactor Type	Fixed Bed	Reactor Type	Fixed Bed
For Fixed Bed reactor type, please choose options below		**For Fixed Bed reactor type, please choose options below**	
Estimated Yearly Resin Loss (%)	0	Estimated Yearly Resin Loss (%)	0
How often the resin is cleaned with NaOH (years)	0	How often the resin is cleaned with NaOH (years)	0
For Mixed reactor type, please choose options below		**For Mixed reactor type, please choose options below**	
Regeneration Ratio (%)	0	Regeneration Ratio (%)	0
Resin Concentration in Ion Exchange Reactor (ml/L)	0	Resin Concentration in Ion Exchange Reactor (ml/L)	0
Resin Concentration in Regeneration Reactor (ml/L)	0	Resin Concentration in Regeneration Reactor (ml/L)	0

Figure 5.2: Screen capture of the comparison tab in the SION simulator, which allows for comparing two different scenarios

5.3 Objective 3: Surveys to Develop a Weighting Scheme for a Sustainability Assessment Framework

In an effort to better assess and compare the sustainability of water treatment in the future, a sustainability assessment framework (SAF) with a semi-quantitative matrix was developed previously and was revised here with stakeholder feedback. This framework can be applied to ion exchange technology, but can also be more widely applied to other water treatment technologies. Rating scale questions have be developed for five “Dimensions”, including technical, environmental, economic, societal and managerial. These are considered across the life cycle stages of technologies including construction, operation & maintenance, and end-of-life. The current version of the SAF is included for reference in Chapter 5’s supplementary information section.

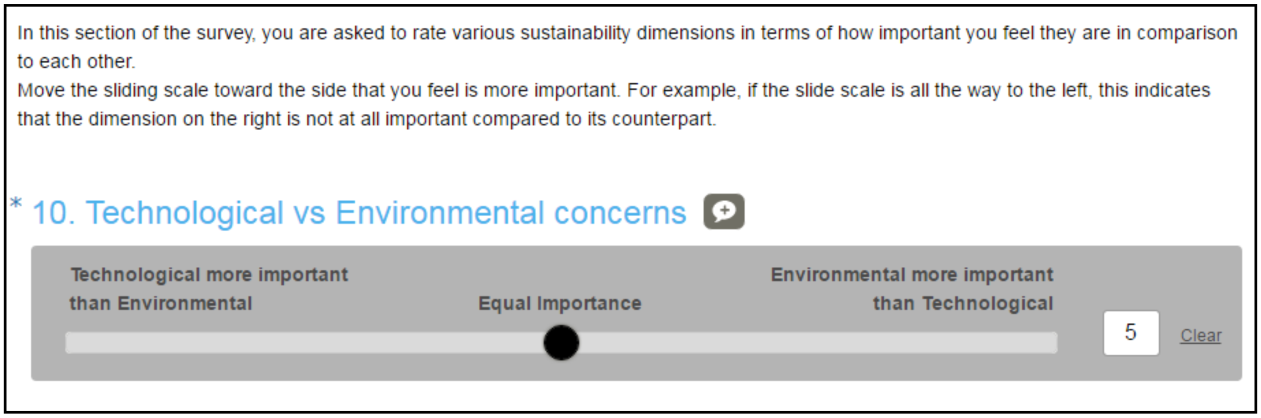
The technological Dimension includes questions related to performance, robustness, ability to be implemented, and transferability, adaptability, and reliability. The environmental Dimension includes questions related to energy use, chemical use, land required, and waste generation and treatment. The economic Dimension addresses questions related to technology costs and externalities. The societal Dimension includes the questions related to risk, acceptance, and ease of use. The managerial Dimension addresses questions related to mechanisms for monitoring, information dissemination, and adaptability. These comprise a total of 18 “Criteria”. Each of these Criteria include qualitative and quantitative indicators. For example, within technical performance are quantitative indicators such as “percentage removal of nitrogenous compounds” and “percentage removal of organic carbon”. There are also qualitative indicators such as, “Can the community/workforce provide sufficient labor and experts?”

A score for each Dimension is normalized by the maximum possible value in that Dimension and a weighting scheme has been developed through the analytic hierarchy process (AHP) (Saaty, 1987). In order to perform the AHP to develop the weighting scheme, a survey was developed and distributed among water professionals asking them to rate the relative importance of the various Criteria of the SAF. AHPs are one of the most popular comprehensive methods for multi-criteria decision analysis and are often used in sustainability planning (Pohekar and Ramachandran, 2004; Wang et al., 2009).

5.3.1 Survey Design

The survey was put into a digital platform with Surveymonkey software in order to make it easy to distribute and complete. Particular attention was given to ensuring that the survey was streamlined, easy to understand, and easy to complete. Feedback was sought from researchers who have had experience with similar surveys and the survey was tested among individuals with various levels of computer literacy.

The survey was designed with three primary sections. The first section collected demographic and background information, such as age, gender, race, current position, experience, and so on. The second section included a pairwise comparison of the five Dimensions of the SAF. Therefore, participants were asked to rate the relative importance of the each of the Dimensions compared to each of the others. This was provided in a format that was easy to understand through a graphical representation. For example, to perform a pariwise comparison of the technical requirements of a treatment plant vs. the environmental requirements, the name “Technical” would be placed on the left and the name “Environmental” would be place on the right, with a sliding scale in between them. The participant was then asked so slide the scale closer toward the side that they feel is more important among the two options. When the slider is in the middle, it indicates that they are of equal importance. The points along the sliding scale correlate to numbers from 0 to 10. For example, 0 would mean that the technical Dimension was strongly more important than the environmental Dimension, 5 would mean that they have equal importance, and 10 would indicate that the environmental Dimension is strongly more important that the technical Dimension. A snapshot showing a portion of this section of the survey is shown below in Figure 5.3.

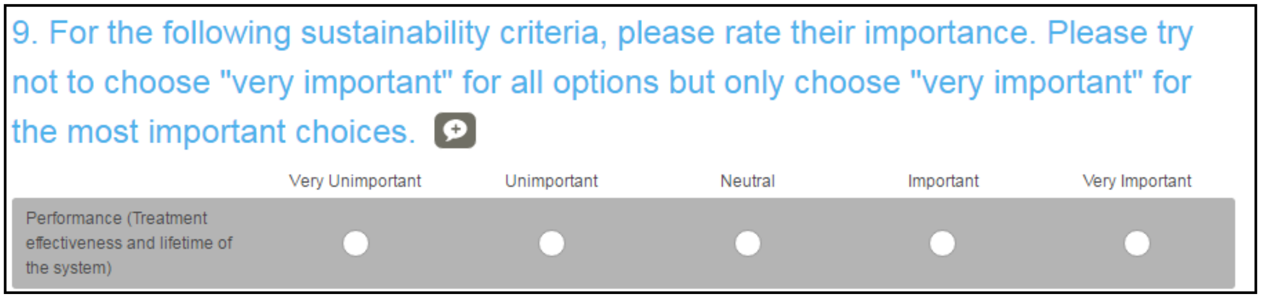


In this section of the survey, you are asked to rate various sustainability dimensions in terms of how important you feel they are in comparison to each other.
Move the sliding scale toward the side that you feel is more important. For example, if the slide scale is all the way to the left, this indicates that the dimension on the right is not at all important compared to its counterpart.

* 10. Technological vs Environmental concerns

Figure 5.3: Snapshot of section 2 of the survey, showing pairwise comparison of dimensions

The third section of the survey allowed for rating of the 18 Criteria. Each of these Criteria fall within one of the 5 Dimensions. Therefore, this allows for more detailed understanding of the values of participants in regards to specific part of the Dimension, possibly allowing for more accurate results. Due to the large number of Criteria and in order to make the survey easier for participants to complete, a pairwise comparison was not used. Instead a simple 1 to 5 rating for each Criteria was used: 1 meaning that the Criteria is unimportant, 3 meaning it is of neutral importance, and 5 meaning that it is very important. A snapshot of section 3 of the survey is shown below in Figure 5.4. A copy of the entire survey is also included in the Chapter 5 supplementary information.



9. For the following sustainability criteria, please rate their importance. Please try not to choose "very important" for all options but only choose "very important" for the most important choices.

	Very Unimportant	Unimportant	Neutral	Important	Very Important
Performance (Treatment effectiveness and lifetime of the system)	○	○	○	○	○

Figure 5.4: Snapshot of section 3 of the survey, showing the criteria rating portion

5.3.2 Survey Distribution and Response

The survey was primarily distributed in electronic format; however, paper surveys were used for six water treatment plants in Florida who were also participants in the research presented in Chapter 2. The target audience of the survey was individuals with employment that relates to water treatment plants. This can include a number of water professionals such as treatment plant operators, superintendants, and other managers of water utilities. In order to distribute the electronic surveys, a number of resources were utilized. The survey was posted in wateroperator.org with a short article describing its purpose and asking water professionals to participate. A number of agencies for environmental protection at the state level were also contacted by email or phone and asked to share the survey among listservs of operators or other water professionals. Furthermore, contact information for water operators and other water professionals was collected from open online databases. From among the open online databases, email addresses and listservs for operators and water professionals were acquired from several states including Oregon, Oklahoma, Massachusetts, North Carolina, and New York. In total, it is expected that the survey was distributed to approximately 3,000 individuals. In order to encourage participation in the survey, a $50 gift card raffle was offered.

The total number of participants of the survey was 83, which was approximately a 3% response rate. Of these 83 participants, all 83 completed section 1, 72 completed sections 1 and 2, and 67 completed all three sections. While this is a significant number of responses, due to the nature of the distribution of the survey and the response rate, the survey results may not provide an entirely representative picture of the views of operators throughout the United States. In order to provide this, a much more comprehensive effort would be needed to engage high numbers of water professionals, which is beyond the scope of the current research. This data provides an initial set of results to develop a weighting scheme for the SAF and allows future researchers to build upon the experience developed in this research in order to better evaluate the sustainability of ion exchange and other water treatment technologies in the future.

5.3.3 Survey Results

5.3.3.1 Section 1 of the Survey

Section 1 of the survey results focused mainly on demographic and background information of the participants. The average age of respondents was 49, with a standard deviation of 10 years, a maximum of 66, and a minimum of 22 years of age. 76% of the respondents were male, 7% were female, and the remaining chose not to report. The respondents were 90% White, approximately 3.5% Native American, approximately 3.5% Hispanic, approximately 1% African American, and approximately 2.5% other races or mixed. Therefore, the majority of respondents were white middle-aged males, which may be typical of water professionals.

The position held by the respondents consisted of 54% operators, 31% Managers, Supervisors, and Superintendents, 2% President/Owners, and 12% other positions such as scada technician or program analyst. Therefore, the majority of respondents were operators and managers of water utilities.

The number of employees at the treatment plant of the respondent averaged at 8.5 employees, with a standard deviation of 10.3, a maximum of 50 employees, and a minimum of 0 (likely for individuals who are not currently at a treatment plant). The size of the plant the respondent works at was an averaged of 12.9 MGD, with a standard deviation of approximately 20 MGD, a max of 120 MGD, and a minimum of 0 MGD. The survey respondents therefore primarily have experience with larger treatment plants and results may be biased toward these larger plants. Water professionals at smaller treatment plants are likely to be more difficult to reach with such surveys because often the operators lack a high degree of technical or computer skills and may not regularly access email. In order to reach smaller plants with this survey, a more intensive effort would likely be required to personally more of these plants and ask operators to participate in this survey. However, this may not be practical in most cases.

In regards to the educational background of the respondents, all have at least received a GED or a high school diploma and none have pursued or completed a Ph.D. Most had a high school education or varying degrees of college education. The results showing the highest level of education they have received is shown in table 5.1 below.

Table 5.1: Self reported highest level of education achieved by survey participants

Highest Level of Education Received	Percentage of Respondents
Did not graduate from High School	0.0%
GED	4.8%
High School Diploma	19.3%
1 year of college	13.3%
2 years of college	27.7%
3 years of college	9.6%
Graduated from college	22.9%
Some graduate school	0.0%
Completed Master's	2.4%
Pursuing PhD	0.0%
Completed PhD	0.0%

5.3.3.2 Section 2 of the Survey

Section 2 of the survey focused on the pairwise comparison of Dimensions, including technical, environmental, economic, societal, and managerial. As described above, the data was scored from 0 to 10 by the participants using a sliding scale to indicate preference of each Dimension over the other. The average of these values was then converted to Saaty’s scale to be used in the analytical hierarchy process (AHP) (Saaty, 1987). Therefore, 0 correlates to 9 (much more important), 5 correlates to 1 (equal importance), and 10 correlates to 1/9 (much less importance) on Saaty's rating scale. The weights were calculated for each Dimension and are shown in Table 5.2. These weights are the main result of the AHP and can be utilized in the SAF for give relative importance to each of the Dimensions. The environmental Dimension was given the greatest preference and weight by participants, followed by the technical Dimension and the economic. The Dimension given the lowest importance was the societal Dimension. The consistency index (CI) for the data was 0.012 and the consistency ratio (CR) was 0.01. This indicates high consistency among the results. The CR is generally required to be below 0.1 to show reliable consistency. Otherwise there can be issues with the data. For example, if the data showed that respondents said item A is much more important than item B and item B is much more important than item C, but item A is only slightly more important than item C, this would be inconsistent data and the CR would be over 0.1.

Table 5.2: Weights for each dimension of the SAF, as calculated by the AHP

Dimension	**Weight**
Technical	21.5%
Environmental	34.5%
Economic	17.7%
Societal	11.3%
Managerial	15.0%

Providing the highest rating for the environmental dimensions shows that the respondents highly value the environmental aspects of water treatment. However, the concept of the environmental is one that is often vague and can be conceptualized in a number of ways. Furthermore, the influence of modern-day media may affect perceptions of the "environment" in a positive way, increasing the perceived value of this dimension. Therefore, the following section focuses on the criteria within each dimension to possible provide a more accurate representation of the respondents values regarding the SAF elements.

5.3.3.3 Section 3 of the Survey

Section 3 of the survey asked respondents to evaluate the importance 18 Criteria that are part of the SAF. These Criteria each fall into one of the sustainability Dimensions. For example, performance, reliability, and robustness all fall within the Technical Dimension. Therefore, these provide a much more specific and detailed understanding of the participants views of the Dimensions of the SAF. Each Criteria was given a rating of 1 to 5. The difference in rating was calculated between all of the pairs of Criteria and this difference was then converted to Saaty's scale of 9 to 1/9 to perform the AHP. The weights calculated for each of the Criteria are shown below in Table 5.3. The highest weight was given to performance of the water treatment technology, with a weight of 14%, followed by reliability (12.8%), and robustness (9.2%). The CI was 0.017 and the CR was 0.01, indicating high consistency among the results.

Although in section 2 the respondents showed a preference for the environmental Dimension, in this section of the survey they clearly showed preference for Criteria that fall in the technical and societal Dimensions. This seems more reasonable than the results of the previous section because it relates to how well the system works and how easy it is to use, which more directly affect the water professionals. The difference between these results and the previous section is likely because the names and descriptions of the Criteria were much more specific that the description of the Dimensions. This seems to indicate that the participants value the general idea and concept of environmental considerations during water treatment, likely due to increased public awareness of the importance of the environment. However, when presented with more specific descriptions of the Criteria, however, the participants tended to favor the Criteria that more directly affect the day-to-day reality at water treatment plants. Therefore, it is likely that the weights of the Criteria are generally more representative of the true values of the participants as compared to the weights for the Dimensions. In applying these weights in the SAF, it is therefore recommended that the weights of the Criteria be used instead of the weights calculated for the Dimensions.

Table 5.3: Weight results of the SAF criteria

Criteria	**Weight**
Performance (Treatment effectiveness and lifetime of the system)	14.0%
Robustness (Endure shock loads and seasonal effects. Ability to cope with fluctuations in influent)	9.2%
Ability to be implemented (Ease of construction)	3.8%
Transferability (Possibility to transfer to another region or system)	1.3%
Adaptability (Possibility to implement in various scales and sizes. Ability to retrofit)	3.3%
Reliability (Sensitivity to malfunctioning of equipment)	12.8%
Energy Usage Amount	5.5%
Chemical Usage Amount	3.9%
Land Area Required	2.0%
Waste Production and Generation (Gas wastes (including as greenhouse gases), liquid wastes, solid wastes)	2.1%
Technology Costs (Cost effectiveness, Affordability)	5.5%
Technology Externality Costs (Cost of regulatory compliance. Economic benefit from resource recovery).	3.6%
Ease of Use	6.7%
Risk Awareness (How aware managers and customers are of the risks of the technology)	3.8%
Acceptance (How willing managers and customer are to accept the technology and the risk)	5.9%
Managerial Mechanisms (Level of automation and data management. Plans to repair and replace components. Emergency response plans.)	7.8%
Information dissemination (Providing information to tour visitors. Providing information on an official website)	2.4%
Managerial Adaptability (Does the workforce have sufficient labor and experts. Do stakeholders understand the technology and support it. Are there available resources to satisfy system requirements)	6.6%

5.4 Conclusion

A disconnect between research and practice has long been recognized (Bero et al., 1998; Buckley et al., 1998; McCown, 2001; Bansal et al., 2012; Langrall, 2014), which limits the broader impact of research. Methods for bridging this gap must not only communicate results to the practitioner community, but also require a collaborative and reciprocal process where the researchers and practitioners learn from each other. This chapter allowed for the research conducted in the previous tasks to be connected more directly to the community of practice by communicating results directly to them, translating the research results into tools that they can utilize, and taking into account their values in the development of new sustainability assessment tools for water treatment technology.

5.5 Acknowledgements

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5.6 References

Arches, J. (1999). Challenges and Dilemmas in Community Development. Journal of Community Practice, 37-55.

Argyris, C., & Schon, D. (1974). Theory in practice: Increasing professional effectiveness. San Francisco: Jossey-Bass.

Bansal, P., Bertels, S., Ewart, T., Macconnachie, P., & O'brien, J. (2012). Bridging the Research-Practice Gap. Academy of Management Perspectives, 73-92.

Bero, L., Grilli, R., Grimshaw, J., Harvey, E., Oxman, A., & Thomson, M. (1998). Getting research findings into practice: Closing the gap between research and practice: An overview of systematic reviews of interventions to promote the implementation of research findings. BMJ, 465-468.

Buckley, M., Ferris, G., Bernardin, H., & Harvey, M. (1998). The disconnect between the science and practice of management. Business Horizons, 31-38.

Langrall, C. (2014). Linking Research and Practice: Another Call to Action? Journal for Research in Mathematics Education, 45(2), 154-156.

McCown, R. (2001). Learning to bridge the gap between science-based decision support and the practice of farming: Evolution in paradigms of model-based research and intervention from design to dialogue. Australian Journal of Agricultural Research, 52, 549–571-549–571.

Pohekar, S., & Ramachandran, M. (2004). Application of multi-criteria decision making to sustainable energy planning—A review. Renewable and Sustainable Energy Reviews, 8(4), 365-381. doi:10.1016/j.rser.2003.12.007

Saaty, R. W. (1987). The analytic hierarchy process—what it is and how it is used. Mathematical Modelling, 9(3-5), 161-176. doi:10.1016/0270-0255(87)90473-8

Wang, J., Jing, Y., Zhang, C., & Zhao, J. (2009). Review on multi-criteria decision analysis aid in sustainable energy decision-making. Renewable and Sustainable Energy Reviews, 13(9), 2263-2278. doi:10.1016/j.rser.2009.06.021

5.7 Chapter 5 Supplementary Information

Below is shown the main portions of the Dimensions, Criteria, and indicators of the current version of the sustainability assessment framework being developed for water treatment technology.

Table 5.4: Dimensions, criteria, and indicators of sustainability assessment framework (1/7)

Dimension	Criteria	Aspect	Indicator Inputs	Qualitative/Quantitative indicator	Evaluation approach
Technological	1. Performance	Treatment efficiency Note: selected technologies include: Ferrate treatment, Alum and ferric coagulation, Ion exchange, Natural filtration	Influent/Effluent Organic Carbon Concentration	removal percentage of organic carbon	removal percentage
			Influent Concentration of metals, Effluent Concentration of metals	removal percentage of transition metals	removal percentage
			Concentration of by-products	harmful by-products (e.g. disinfection by-products (DBPs))	max{ ([BP]ref - [BP])/[BP]ref, 0 }
			Influent/Effluent Concentration of nitrogenous compounds	removal percentage of nitrogenous compounds	removal percentage
			Conc.of oxidizable trace contaminants of emerging concern	oxidizable trace contaminants of emerging concern (pharmaceuticals, personal care products)	removal percentage
			Influent/Effluent Concentration of Particles	removal percentage of particles	removal percentage

Table 5.5: Dimensions, criteria, and indicators of sustainability assessment framework (continued 2/7)

Dimension	Criteria	Aspect	Indicator Inputs	Qualitative/Quantitative indicator	Evaluation approach
Technological	1. Performance	Treatment efficiency	Influent Concentration of Pesticides, Effluent Concentration of Pesticides	removal percentage of selected pesticides	removal percentage
		Durability	Life time	Life time	[life time]/[life time]ref
	2. Robustness	Endure shock loads/seasonal effects	Time	the time to recover to normal treatment efficiency	max{ ([time]ref - [time])/[time]ref, 0 }
		Ability to cope with fluctuations in the influent	Standard deviation of effluent quality, Standard deviation of influent quality	ratio of the standard deviation of effluent quality to the standard deviation of influent quality	1 - σ_in / σ_eff
	3. Ability to be implemented	Ease of construction	Time	the time to construct	max{ ([time]ref - [time])/[time]ref, 0 }
			Hours of labor	the labor needed for construction	max{ ([labor #]ref - [labor #])/[labor #]ref, 0 }
	4. Transferability	Possibility to transfer to another region or system	Rated Survey	Difficulty in implementing the technology based on the required regulatory procedure	qualitative
			# Systems	the number of systems using this tech and potential systems willing to adopt this tech	[system #]/[system #]_ref

Table 5.6: Dimensions, criteria, and indicators of sustainability assessment framework (continued 3/7)

Dimension	Criteria	Aspect	Indicator Inputs	Qualitative/Quantitative indicator	Evaluation approach
Technological	4. Transferability	Possibility to transfer to another region or system	# States	the number of states or counties using this tech.	[state #]/[state #]_ref
	5. Adaptability	Possibility to implement the technology in various scales	Scale range	the span of the capacity scale range	[span]/[span]_ref
		Ability to retrofit	Rated Survey	Ease of retrofitted existing system	qualitative
	6. Reliability	Sensitivity of the technology to malfunctioning of equipment and instrumentation	Standard effluent quality, Effluent quality during malfunction	the change of treatment efficiency or effluent water quality when essential equipment malfunction	1 - [treatment efficiency change]
Environmental	1. Energy use	Energy consumption rate	kWh of Electricity Consumed, Flow rate	electricity consumed per 1000 gallon treated water	max{ ([E]ref - [E])/[E]ref, 0 }
	2. Chemical use	Chemical use rate	Name and mass of chemicals	mass and type of chemical used per 1000 gallon treated water	max{ ([M]ref - [M])/[M]ref, 0 }
	3. Land required	Land area required	Land area, Flow rate	land area required divide by treatment capacity	max{ ([X]ref - [X])/[X] ref, 0 }
	4. Waste generation and treatment	Gas waste, such as GHG emission	Volume of GHG emissions, Flow rate	volume of GHG emission per 1000 gallon treated water	max{ ([X]ref - [X])/[X] ref, 0 }
		Liquid waste (residual stream)	Name and volume of liquid waste, Flow rate	volume and type of liquid waste per 1000 gallon treated water	max{ ([X]ref - [X])/[X] ref, 0 }

Table 5.7: Dimensions, criteria, and indicators of sustainability assessment framework (continued 4/7)

Dimension	**Criteria**	**Aspect**	**Indicator Inputs**	**Qualitative/Quantitative indicator**	**Evaluation approach**
Environmental	4. Waste generation and treatment	Liquid waste (residual stream)	Concentration	concentrations in liquid waste	max{ ([X]ref - [X])/[X]ref, 0 }
		Solid waste	Name and mass of solid waste, Flow rate	mass and type of solid waste per 1000 gallon treated water	max{ ([X]ref - [X])/[X]ref, 0 }
Economic	1. Technology costs	Cost effectiveness	Capital Cost, Operation & Maintenance cost per month or year, Flow rate, Influent Concentration of Contaminant, Effluent Concentration of Contaminant	total cost divided by (treated water volume multiply effluent quality)	max{ ([X]ref - [X])/[X]ref, 0 }
		Affordability	Standard Water Bill, Water Bill with New Technology, Household monthly income	the change of regular household water bill (water rate multiply volume used by a regular family) caused by implementing new tech. divided by household monthly income	1 - change/regular bill

Table 5.8: Dimensions, criteria, and indicators of sustainability assessment framework (continued 5/7)

Dimension	**Criteria**	**Aspect**	**Indicator Inputs**	**Qualitative/Quantitative indicator**	**Evaluation approach**
Economic	2. Technology externality	Cost of Regulatory Compliance	Regulatory Compliance Cost, Total Cost (Capital and Operating Expenses)	the ratio of hidden cost to total cost	1 - X
		Economic benefit from resource recovery	Cost savings/profit from resource recovery, Total Cost (Capital and Operating Expenses)	the ratio of economic benefit from resource recovery to total cost	X
Societal	1. Risk	Awareness of risk	Rated Survey	how aware are managers of the risk of adding this tech?	qualitative
			Rated Survey	how aware are customers of the risk of adding this tech?	qualitative
	2. Acceptance	Acceptance of technology and risk	Rated Survey	how willing are the managers to accept this tech and take the risk?	qualitative
			Rated Survey	how willing are the customers to accept this tech and take the risk?	qualitative
	3. Ease of use	Competence/information requirements	Rated Survey	can typical users without training for the specific equipment understand it and know how to operate?	qualitative

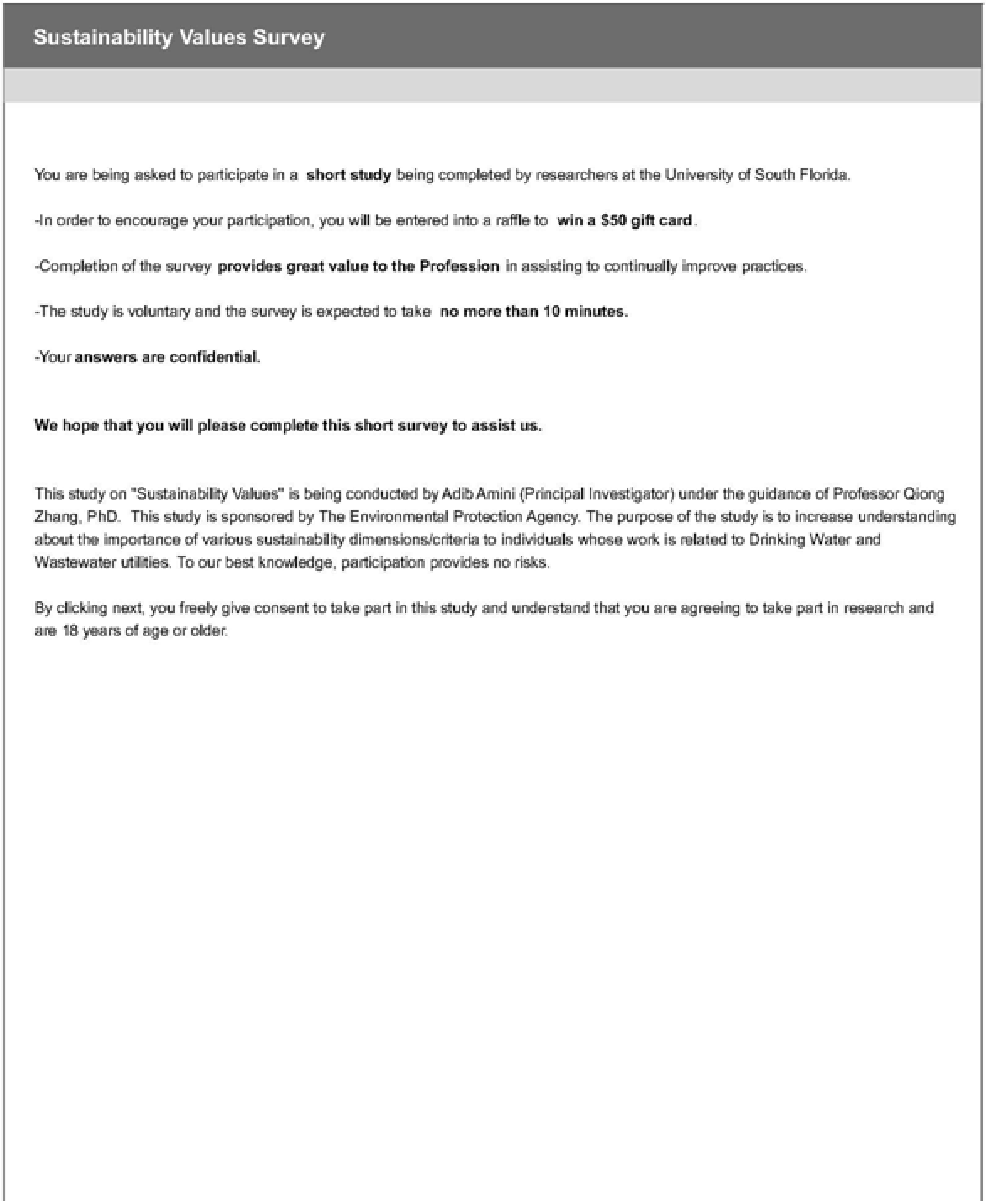
Table 5.9: Dimensions, criteria, and indicators of sustainability assessment framework (continued 6/7)

Dimension	Criteria	Aspect	Indicator Inputs	Qualitative/Quantitative indicator	Evaluation approach
Managerial	1. Mechanism	Mechanisms for monitoring	Rated Survey	how is water quality being monitored (automatically, semi-automatically, or manually)	qualitative
		Operational Optimization when implementing the tech into system	Rated Survey	have different operation strategies been tested and simulated to minimized resource use, loss, and impacts?	qualitative
		Infrastructure Stability	Rated Survey	is there a plan in place to repair and replace the components needed for the technology	qualitative
		Operational Resiliency	Rated Survey	has a vulnerability assessment been conducted for safety, natural disasters, and other environmental threats?	qualitative
			Rated Survey	is an emergency response plan prepared for these hazards?	qualitative
	2. Information dissemination	Information dissemination methods	Rated Survey	is the tech introduced in the tour of visitors?	qualitative
			Rated Survey	is the information of the tech included in the official website?	qualitative

Table 5.10: Dimensions, criteria, and indicators of sustainability assessment framework (continued 7/7)

Dimension	**Criteria**	**Aspect**	**Indicator Inputs**	**Qualitative/Quantitative indicator**	**Evaluation approach**
Managerial	3. Adaptability	Labor and expert adequacy	Rated Survey	can the community/workforce provide sufficient labor and experts?	qualitative
		Stakeholder understanding & support	Rated Survey	do stakeholders understand the tech and support it?	qualitative
		Resource adequacy	Rated Survey	do the available resources satisfy the needs of the tech?	qualitative

Below is the content of the survey developed and distributed to develop a weighting scheme for the sustainability assessment framework.



Sustainability Values Survey

You are being asked to participate in a **short study** being completed by researchers at the University of South Florida.

-In order to encourage your participation, you will be entered into a raffle to **win a $50 gift card**.

-Completion of the survey **provides great value to the Profession** in assisting to continually improve practices.

-The study is voluntary and the survey is expected to take **no more than 10 minutes.**

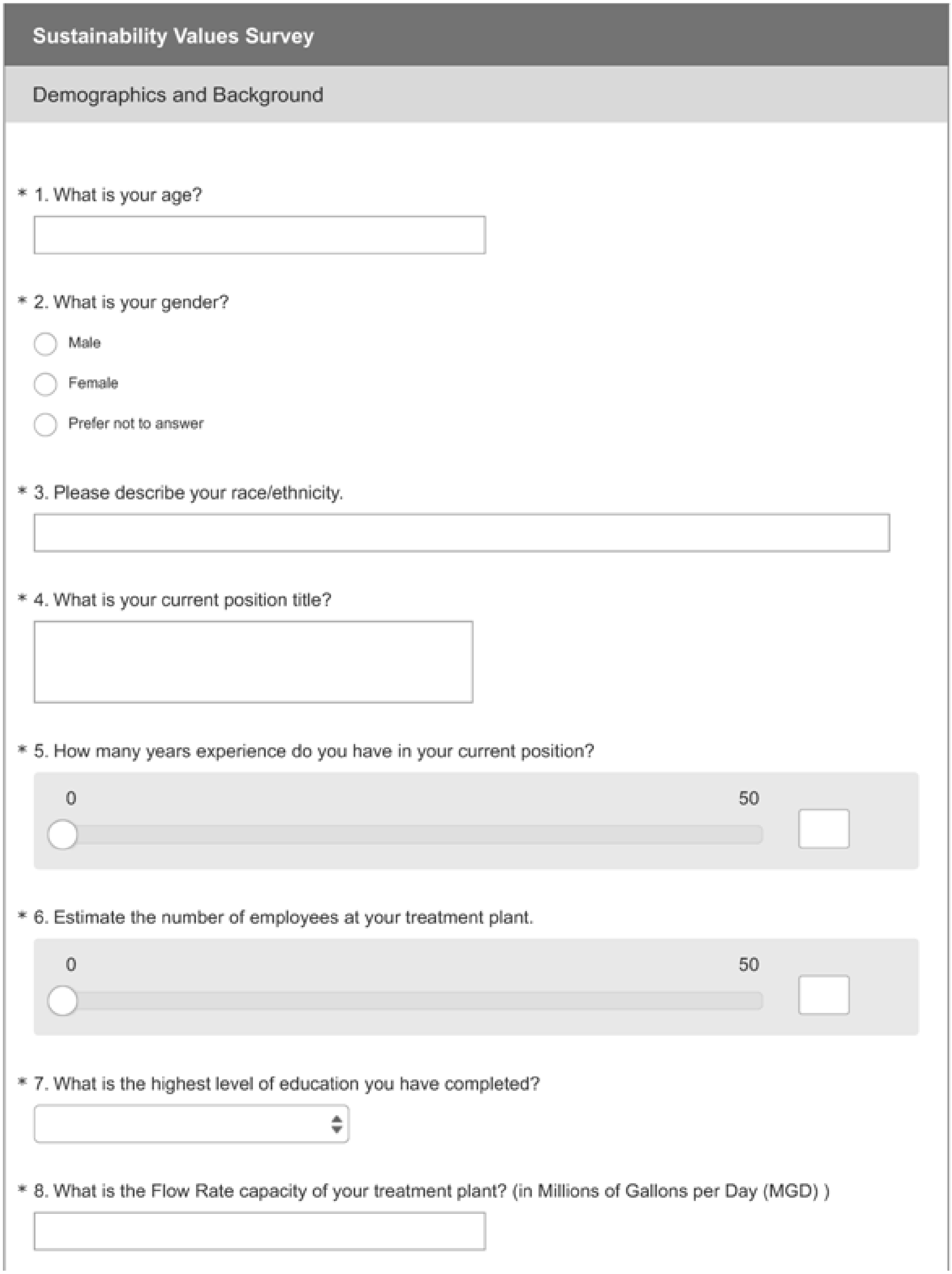
-Your **answers are confidential.**

We hope that you will please complete this short survey to assist us.

This study on "Sustainability Values" is being conducted by Adib Amini (Principal Investigator) under the guidance of Professor Qiong Zhang, PhD. This study is sponsored by The Environmental Protection Agency. The purpose of the study is to increase understanding about the importance of various sustainability dimensions/criteria to individuals whose work is related to Drinking Water and Wastewater utilities. To our best knowledge, participation provides no risks.

By clicking next, you freely give consent to take part in this study and understand that you are agreeing to take part in research and are 18 years of age or older.

Figure 5.5: Copy of survey given to water professionals (page 1)



Sustainability Values Survey

Demographics and Background

* 1. What is your age?

* 2. What is your gender?

○ Male

○ Female

○ Prefer not to answer

* 3. Please describe your race/ethnicity.

* 4. What is your current position title?

* 5. How many years experience do you have in your current position?

0 50

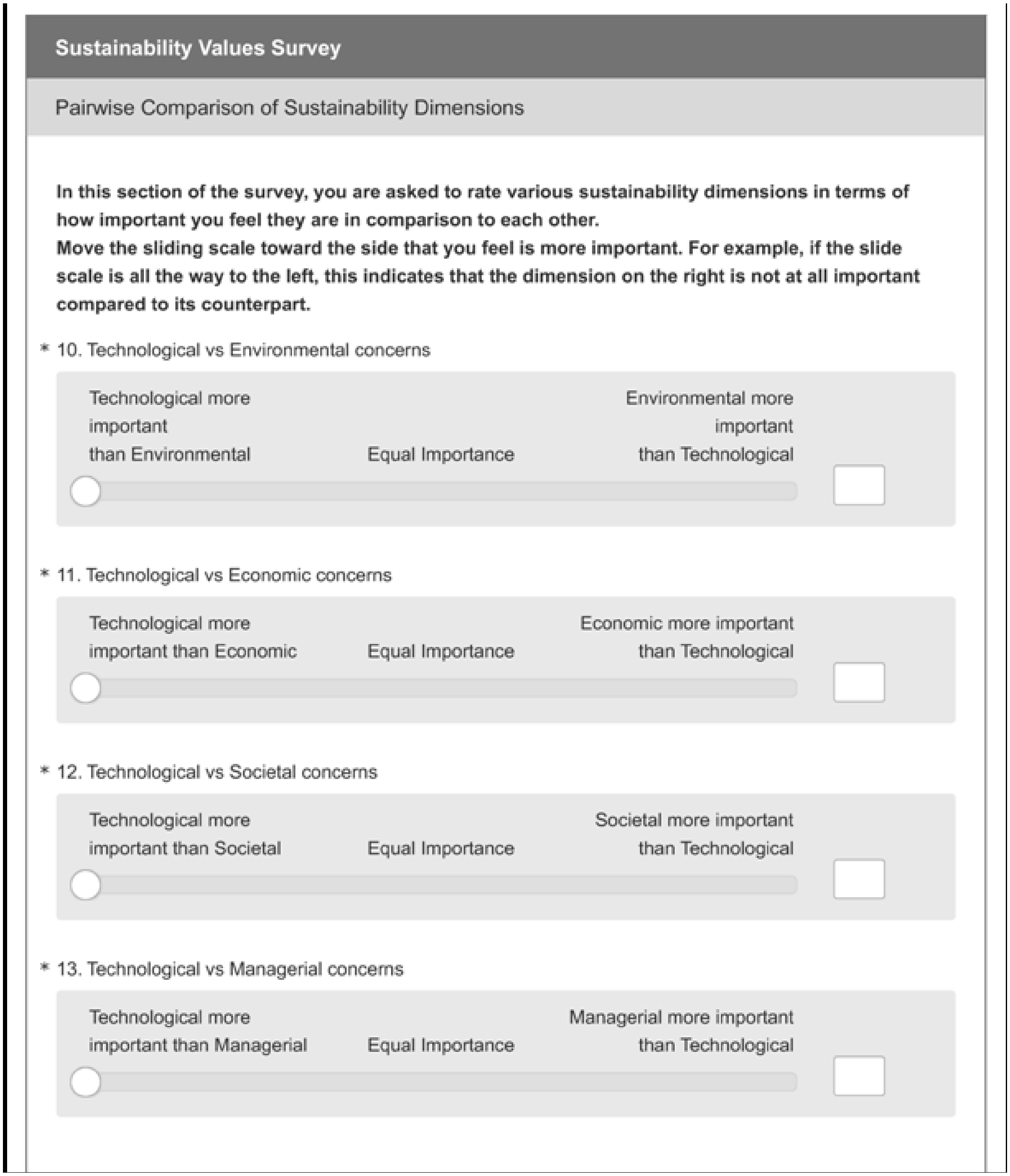
* 6. Estimate the number of employees at your treatment plant.

0 50

* 7. What is the highest level of education you have completed?

* 8. What is the Flow Rate capacity of your treatment plant? (in Millions of Gallons per Day (MGD))

Figure 5.6: Copy of survey given to water professionals (page 2)



Sustainability Values Survey

Pairwise Comparison of Sustainability Dimensions

In this section of the survey, you are asked to rate various sustainability dimensions in terms of how important you feel they are in comparison to each other.
Move the sliding scale toward the side that you feel is more important. For example, if the slide scale is all the way to the left, this indicates that the dimension on the right is not at all important compared to its counterpart.

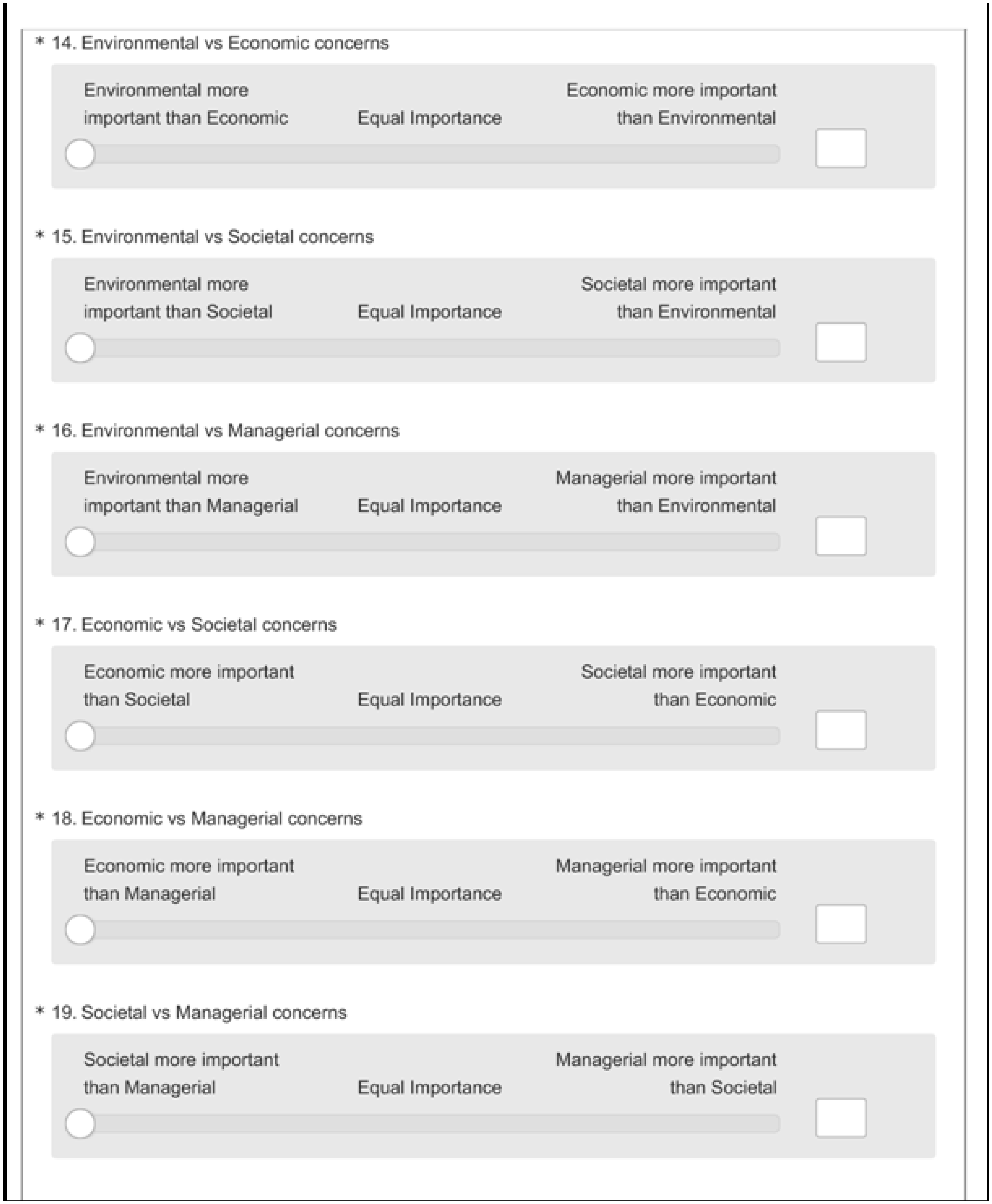
* 10. Technological vs Environmental concerns

* 11. Technological vs Economic concerns

* 12. Technological vs Societal concerns

* 13. Technological vs Managerial concerns

Figure 5.7: Copy of survey given to water professionals (page 3)



* 14. Environmental vs Economic concerns

Environmental more important than Economic | Equal Importance | Economic more important than Environmental

* 15. Environmental vs Societal concerns

Environmental more important than Societal | Equal Importance | Societal more important than Environmental

* 16. Environmental vs Managerial concerns

Environmental more important than Managerial | Equal Importance | Managerial more important than Environmental

* 17. Economic vs Societal concerns

Economic more important than Societal | Equal Importance | Societal more important than Economic

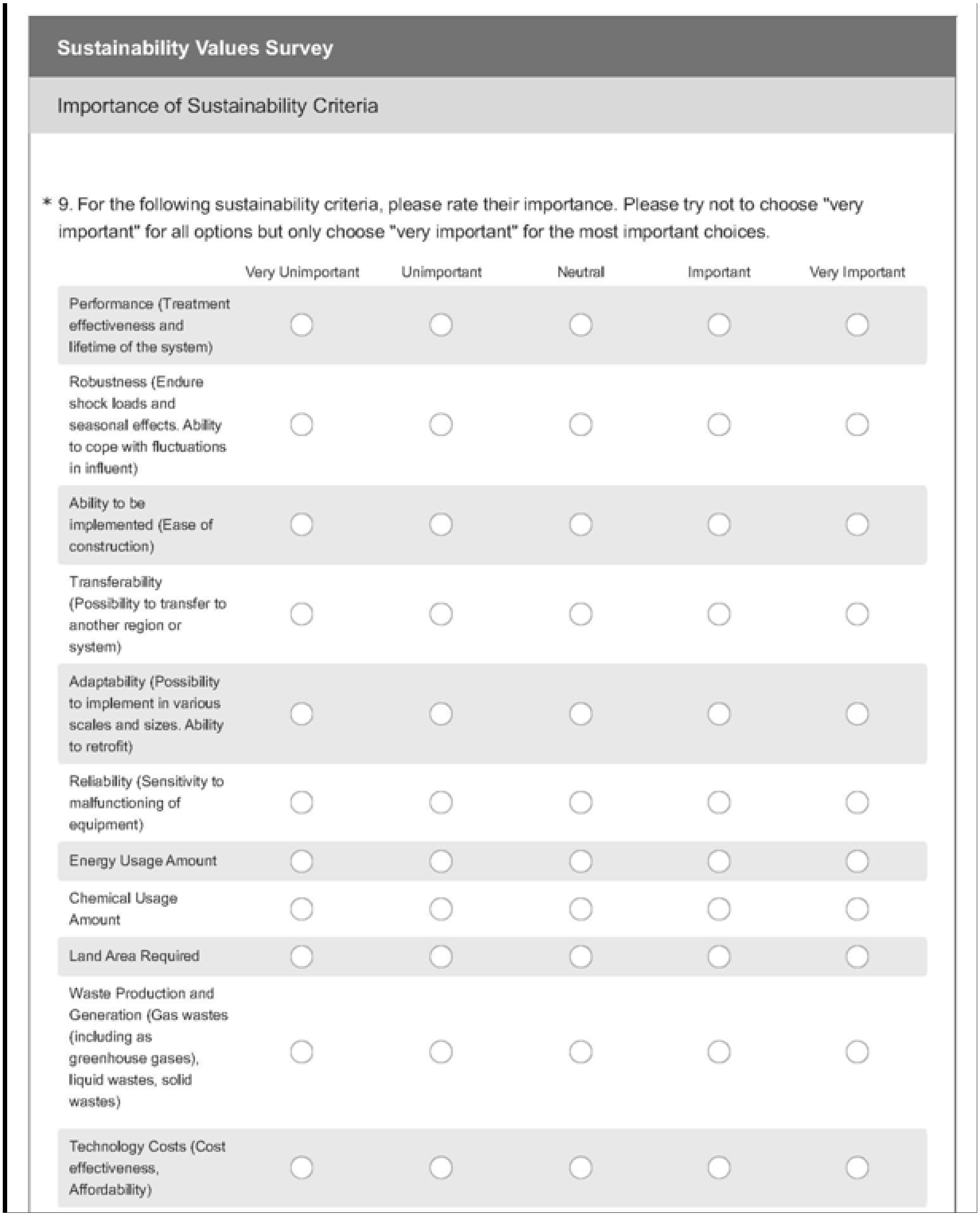
* 18. Economic vs Managerial concerns

Economic more important than Managerial | Equal Importance | Managerial more important than Economic

* 19. Societal vs Managerial concerns

Societal more important than Managerial | Equal Importance | Managerial more important than Societal

Figure 5.8: Copy of survey given to water professionals (page 3 continued)



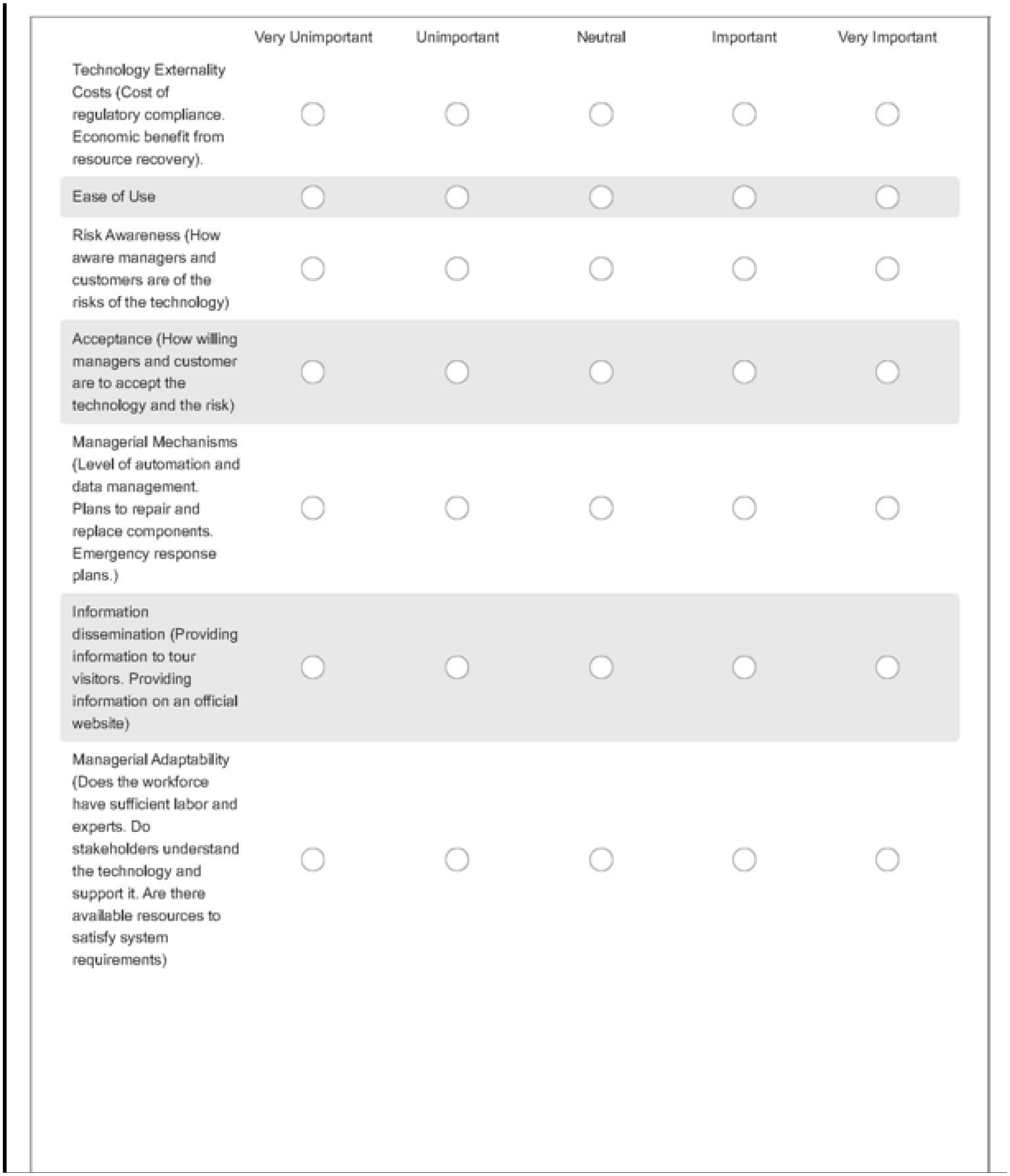
Sustainability Values Survey

Importance of Sustainability Criteria

* 9. For the following sustainability criteria, please rate their importance. Please try not to choose "very important" for all options but only choose "very important" for the most important choices.

	Very Unimportant	Unimportant	Neutral	Important	Very Important
Performance (Treatment effectiveness and lifetime of the system)	○	○	○	○	○
Robustness (Endure shock loads and seasonal effects. Ability to cope with fluctuations in influent)	○	○	○	○	○
Ability to be implemented (Ease of construction)	○	○	○	○	○
Transferability (Possibility to transfer to another region or system)	○	○	○	○	○
Adaptability (Possibility to implement in various scales and sizes. Ability to retrofit)	○	○	○	○	○
Reliability (Sensitivity to malfunctioning of equipment)	○	○	○	○	○
Energy Usage Amount	○	○	○	○	○
Chemical Usage Amount	○	○	○	○	○
Land Area Required	○	○	○	○	○
Waste Production and Generation (Gas wastes (including as greenhouse gases), liquid wastes, solid wastes)	○	○	○	○	○
Technology Costs (Cost effectiveness, Affordability)	○	○	○	○	○

Figure 5.9: Copy of survey given to water professionals (page 4)



	Very Unimportant	Unimportant	Neutral	Important	Very Important
Technology Externality Costs (Cost of regulatory compliance. Economic benefit from resource recovery).	○	○	○	○	○
Ease of Use	○	○	○	○	○
Risk Awareness (How aware managers and customers are of the risks of the technology)	○	○	○	○	○
Acceptance (How willing managers and customer are to accept the technology and the risk)	○	○	○	○	○
Managerial Mechanisms (Level of automation and data management. Plans to repair and replace components. Emergency response plans.)	○	○	○	○	○
Information dissemination (Providing information to tour visitors. Providing information on an official website)	○	○	○	○	○
Managerial Adaptability (Does the workforce have sufficient labor and experts. Do stakeholders understand the technology and support it. Are there available resources to satisfy system requirements)	○	○	○	○	○

Figure 5.10: Copy of survey given to water professionals (page 4 continued)

Table 5.11: Raw results of pairwise comparison of dimensions; each line represents an individual response (1/3)

Technological vs Environmental concerns	Technological vs Economic concerns	Technological vs Societal concerns	Technological vs Managerial concerns	Environmental vs Economic concerns	Environmental vs Societal concerns	Environmental vs Managerial concerns	Economic vs Societal concerns	Economic vs Managerial concerns	Societal vs Managerial concerns
5	3	4	4	5	4	5	6	6	4
8	3	3	2	3	3	3	2	2	7
5	3	5	5	7	6	5	5	5	4
9	5	5	5	5	5	5	5	5	5
4	4	4	2	5	5	4	4	4	6
5	5	4	4	5	5	4	5	5	5
5	1	0	5	5	5	5	5	9	5
5	7	7	3	4	4	3	6	4	5
6	6	6	6	4	4	4	6	6	6
9	7	9	8	1	1	1	9	7	8
7	5	4	5	4	4	4	6	5	5
5	4	4	4	5	4	5	4	4	5
7	7	7	3	4	4	4	4	4	4
5	6	5	5	5	4	5	5	5	6
5	5	5	5	5	5	5	5	5	5
2	6	5	5	8	7	5	5	5	5
5	4	5	4	4	4	3	5	5	5
5	5	3	3	5	3	3	5	5	5
5	3	1	10	10	0	10	0	10	10
7	6	4	5	4	5	4	5	5	5
4	6	4	3	5	4	6	2	4	6
6	5	4	6	4	4	4	4	5	6
5	5	4	5	5	5	5	5	5	5
6	4	6	3	4	2	3	4	4	4
6	6	6	6	4	4	4	4	6	6
5	5	5	5	5	5	5	5	5	5
6	7	7	3	3	2	0	2	2	7
6	5	4	3	3	4	4	5	5	5
5	5	5	6	5	5	6	5	6	6
5	6	5	4	5	5	4	5	5	5

Table 5.12: Raw results of pairwise comparison of dimensions; each line represents an individual response (continued 2/3)

Technological vs Environmental concerns	Technological vs Economic concerns	Technological vs Societal concerns	Technological vs Managerial concerns	Environmental vs Economic concerns	Environmental vs Societal concerns	Environmental vs Managerial concerns	Economic vs Societal concerns	Economic vs Managerial concerns	Societal vs Managerial concerns
5	5	4	5	4	5	4	4	4	6
6	4	5	6	4	5	7	5	7	5
5	3	2	2	3	0	2	7	7	3
8	4	4	3	8	3	3	8	3	3
10	3	3	5	4	3	3	3	3	3
5	5	5	5	6	5	6	5	5	5
0	5	0	0	10	5	5	0	0	5
5	2	3	1	9	1	2	8	2	8
10	8	9	3	0	2	0	5	5	4
5	4	2	4	5	4	5	3	5	6
5	3	3	3	6	3	3	3	7	8
5	5	4	5	5	5	5	5	5	5
5	5	2	5	5	5	2	5	5	5
5	5	5	5	5	5	5	5	5	5
5	4	3	5	5	4	4	4	5	5
1	4	7	3	8	5	6	9	8	5
5	5	5	5	4	5	4	5	4	4
7	5	3	6	5	5	5	5	5	7
6	3	6	4	3	3	4	6	6	6
9	8	8	2	2	2	2	2	2	10
7	4	3	5	2	4	4	5	4	4
5	5	5	6	5	5	6	5	6	6
8	6	7	1	1	1	0	9	1	1
9	4	5	5	3	0	3	3	5	5
5	6	6	5	5	5	5	6	5	4
4	7	3	5	6	4	6	3	3	5
6	5	6	5	3	4	4	3	5	5
8	6	6	6	4	5	6	7	5	8
8	5	6	5	3	4	5	4	5	6
4	5	5	6	5	5	6	5	5	5
5	4	4	5	4	4	4	4	5	5

Table 5.13: Raw results of pairwise comparison of dimensions; each line represents an individual response (continued 3/3)

Technological vs Environmental concerns	Technological vs Economic concerns	Technological vs Societal concerns	Technological vs Managerial concerns	Environmental vs Economic concerns	Environmental vs Societal concerns	Environmental vs Managerial concerns	Economic vs Societal concerns	Economic vs Managerial concerns	Societal vs Managerial concerns
5	3	2	8	2	3	2	3	8	8
7	6	3	4	4	4	5	4	5	5
5	5	5	5	3	5	5	5	5	5
5	5	4	5	6	4	6	4	6	6
5	5	5	5	5	5	5	4	5	5
4	4	6	2	4	4	1	4	6	6

Table 5.14: Raw survey results for rating of criteria

	Very Unimportant	Unimportant	Neutral	Important	Very Important
Performance (Treatment effectiveness and lifetime of the system)	4	0	5	27	36
Robustness (Endure shock loads and seasonal effects. Ability to cope with fluctuations in influent)	2	1	8	42	19
Ability to be implemented (Ease of construction)	0	4	26	32	10
Transferability (Possibility to transfer to another region or system)	9	9	31	16	7
Adaptability (Possibility to implement in various scales and sizes. Ability to retrofit)	1	3	29	29	10
Reliability (Sensitivity to malfunctioning of equipment)	3	0	8	29	32
Energy Usage Amount	1	4	17	35	15
Chemical Usage Amount	3	4	18	35	12
Land Area Required	4	8	31	16	13
Waste Production and Generation (Gas wastes (including as greenhouse gases), liquid wastes, solid wastes)	5	9	21	26	11
Technology Costs (Cost effectiveness, Affordability)	2	1	21	32	16
Technology Externality Costs (Cost of regulatory compliance. Economic benefit from resource recovery).	2	2	26	31	11
Ease of Use	3	2	13	35	19
Risk Awareness (How aware managers and customers are of the risks of the technology)	3	1	24	33	11
Acceptance (How willing managers and customer are to accept the technology and the risk)	1	3	17	36	15
Managerial Mechanisms (Level of automation and data management. Plans to repair and replace components. Emergency response plans.)	2	2	15	31	22
Information dissemination (Providing information to tour visitors. Providing information on an official website)	3	9	23	26	11
Managerial Adaptability (Does the workforce have sufficient labor and experts. Do stakeholders understand the technology and support it. Are there available resources to satisfy system requirements)	1	3	16	35	17

Chapter 6: Conclusions and Future Research Recommendations

6.1 Conclusions

This research investigated using a life cycle environmental and economic approach to evaluate IX technology for small potable water systems, allowing for the identification and development of process and design improvements that reduce environmental impacts and costs. The main goals were to: evaluate conventional IX in terms of life cycle environmental and economic sustainability, develop a method for design improvement of IX systems through a environmental and economic sustainability perspective, evaluate design improvements, such as combined IX removal, and make the research findings accessible to water professionals through user-friendly tools that can be used in the field as well as assessment frameworks. The conclusions drawn from this work can be summarized as follows.

6.1.1 Task 1

- The environmental impacts of the operation phase of IX treatment is significantly greater than the impacts due to the construction phase
- A functional unit that takes into account both water quantity and water quality treated can significantly alter relative assessment results, showing a more fair comparison between the systems studied.
- The two main designs employed for IX systems are a fixed bed reactor (FBR) design and a completely mixed flow reactor (CMFR) design.
    - FBR designs use less electricity, resin, and transport but require more salt and produce more brine waste, primarily because of higher regeneration requirements

    which can be caused by improper maintenance of resins. However, if the resin in FBR systems is maintained well, these systems will have less salt consumption than CMFR systems.

    - FBR designs therefore have higher environmental impact than CMFR systems in areas of eutrophication, carcinogenics, non-carcinogenics, and ecotoxicity when resins are not maintained well, due to increased regeneration requirements. Efforts to improve sustainability of those systems are best directed toward reducing regeneration requirements, which can include period resin cleaning.
    - FBR systems have lower operation cost than CMFR systems because of the relatively low price of salt and brine waste disposal.
    - Conclusions related to the comparison between FBR and CMFR designs, however, may not be generalized when there is no regeneration performed, such as when using selective IX (in which no regeneration is performed)
- Environmental impacts and costs of the operation phase of IX systems per functional unit were found to decrease as scale increases, likely due to higher efficiency of pumping and mixing at larger scales.

6.1.2 Task 2

- A model that integrates process modeling with LCA and LCCA was developed, which allows for design improvement of IX systems
- A genetic algorithm can be used to identify optimal designs with the model
- The model shows that general trends indicate that designing an IX system with an FBR configuration, NaCl as a regenerant, smaller resin sizes, and higher HRTs (if a larger reactor

does not incur significantly higher costs) can reduce the environmental impacts and costs of IX systems.

- For FBR systems, regular resin cleaning every 3 years in FBR systems and low resin attrition reduces impacts and costs.
- For CMFR systems, regeneration ratios of approximately 15%, high resin concentrations in the IX reactor, and lower resin concentrations in the regeneration reactor can provide the lowest costs and impact.
- Taking into account the effect of the brine on biological processes at the WWTP can contribute to approximately 7-20% of lifetime impacts and costs of IX systems.

6.1.3 Task 3

- IX softening systems tend to require more salt, generate more brine, and require more transport than IX DOC systems.
- This translates into lower environmental impacts and operation costs being incurred by DOC removal compared to equivalent softening systems.
- FBR systems tend to generally require less salt, energy, and resin than CMFR systems.
- Although FBR systems generate more brine waste by volume than CMFR systems, the brine is more diluted, which is preferable in preventing shock loads when the waste brine is discharged to the wastewater treatment plant.
- FBR systems have lower impacts and costs than equivalent CMFR systems. Due to the longer lifetime of FBR systems, the capital cost is also effectively lower than CMFR systems.
- Combined cation anion exchange (CCAE) systems can provide advantages to the combination of two separate IX systems.

    - A theoretical CCAE system, which is based in a CMFR design, was found to have lower impacts and costs than a combination of two CMFR systems. However, the system must be properly designed and operated to reuse brine for cation and anion regeneration, which can reduce salt requirements, brine waste generation, and infrastructure requirements.
- Utilizing CCAE with a reactor design that has lower overall impacts and costs, such as an FBR, will further maximize its benefit.

6.1.4 Task 4

- The following were accomplished to help bridge the gap between research and practice.
- The results of the previous tasks were shared directly with stakeholders that participated in provided data for the systems studied.
- A user-friendly tool was developed for evaluating the environmental impacts and costs of IX design scenarios. This makes the research accomplished in previous tasks accessible to water professionals and useful in the field.
- A sustainability assessment framework that takes into account feedback from water professionals is being developed to compare various types of water treatment technology from the perspective of technological, environmental, economic, societal, and managerial sustainability.

6.2 Recommendations for Future Study

A number of efforts could be pursued to further develop and build upon the research that was accomplished in this dissertation.

- While a robust life cycle environmental impact and cost assessment of IX systems that remove DOC was performed in Task 1, this method also needs to be applied to IX systems that remove other types of contaminants because such systems can differ widely in material and energy requirements as well as waste production.

- One of the factors that can limit the use of IX systems is the brine waste production. Therefore, methods for brine reuse or reduction are particularly needed at this time for IX.
- The model developed in Task 2 can be expanded to include more applications of IX. This would overall make it more useful in providing comparisons while also making it much more valuable to engineers and other water professionals
- Use of CCAE technology using a FBR should be investigated more thoroughly, particularly investigating methods to prevent precipitation and clogging of the fixed bed.
- The user-friendly tool developed in Task 4 can be expanded to include more functionality. For example, it can provide more interactive visualization of results. It can also allow for more customization of the system inputs. For example, the tool currently does not allow users to customize options such as the price of salt and electricity that the model assumes. These assumptions can have dramatic differences on the model results.

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