DISSERTATION

VIABILITY AND SUSTAINABILITY OF DESALINATING PRODUCED WATER IN THE OIL AND GAS INDUSTRY

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Brandi M. Grauberger

Department of Mechanical Engineering

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Doctoral Committee:

Advisor: Todd M. Bandhauer
Co-Advisor: Tiezheng Tong

Sybil Sharvelle
Jason C. Quinn

ABSTRACT

VIABILITY AND SUSTAINABILITY OF DESALINATING PRODUCED WATER IN THE OIL AND GAS INDUSTRY

Unconventional oil and gas extraction[1] consumes considerable amounts of water, with up to 11 million gallons of freshwater used for the fracturing of a single well. Millions of gallons can come back to the surface of a well as flowback and produced waters, which are collected and disposed of through deep well injection. Water reallocation and reduction of resource waste can be aided by treating produced water from these operations but is rarely practiced. In particular, treating produced water to zero-liquid-discharge allows for management of dry wastes and generates a clean water source as its only other product. Eliminating the disposal of brines from produced water management would eliminate the need for deep well injection, which has shown to be an unsustainable option for produced water management. A major barrier to produced water treatment is the cost and availability of energy for treatment. Other barriers arise from an incomplete understanding of the system. Specifically, environmental and social impacts of produced water treatment are not understood. For example, it is not known if the discharge of treated produced water will have a negative effect on drinking water supplies or flow of rivers and streams. Without solving these challenges, produced water will continue to be disposed into injection wells, wasting

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[1] Unconventional oil and gas extraction is any extraction which is not traditional vertical extraction. Unconventional oil includes oil obtained through directional drilling and/or through hydraulic fracturing.

the potential to reduce freshwater consumption, and further threatening seismic stability and access to freshwater reserves in oil and gas producing regions.

This work completes three major analyses to understand the potential of produced water desalination. First, the accessibility of waste heat from the oil and gas industry, which is limited due to spatial and temporal disparities in waste heat and produced water production, was quantified and compared to energy requirements for produced water treatment. The results show that there is potential for waste heat utilization by membrane distillation, a thermal-membrane desalination technology option, in the oil and gas industry for produced water desalination with appropriate waste heat storage system integrations. The next major evaluation is of the economic and environmental impacts for multiple zero liquid discharge desalination options. Economic results show that the existing technology of mechanical vapor compression is difficult to reliably challenge, in terms of cost. However, environmental emissions can be much improved when using waste heat as an energy source for desalination or when treating with electrodialytic crystallization. Finally, this work evaluates options for zero liquid discharge desalination in the oil and gas industry using a triple bottom line sustainability framework. This framework considers the economic, environmental, and social competitiveness of technologies in multiple stakeholder-preference scenarios, which weight the importance of the three categories in different ratios. Results show that the use of waste heat is paramount to the consideration of membrane distillation as a technology option in the oil and gas industry. Further results show that the comprehensive consideration of economic, environment, and social impacts provide context to overall fit of technology options in the oil and gas industry. More detail of each major objective of this work are shared in the following paragraphs.

The use of waste heat has been proposed to reduce the energy footprint of membrane distillation for flowback and produced water treatment. However, its feasibility has not been fully understood for produced water treatment. Accordingly, the third chapter of this work performed systematic assessments through thermodynamic modelling of waste heat capture, storage, and transportation for decentralized produced water treatment at well pads located in the Denver-Julesburg Basin. A wide range of sensible, phase-change, and thermo-chemical storage materials were assessed for their effectiveness at the utilization of waste heat from on-site hydraulic fracturing engines and natural gas compressor stations, in order to overcome the temporal or spatial mismatch between waste heat availability and produced water generation. Results show that the type of storage material being used can have a high impact on the efficiency of waste heat utilization and the treatment capacity of membrane distillation. Sensible storage materials only utilize sensible heat capacities, while phase-change materials have improved performance because they are able to additionally store latent heat. However, sensible and phase-change storage materials lose 11–83% of heat due to conversion inefficiencies caused by their changing temperatures. Thermo-chemical materials, on the other hand, have the highest potential for use because they collect and release heat at constant temperatures. Three thermo-chemical storage materials (magnesium sulfate, magnesium chloride, and calcium sulfate) were identified as those with the best efficiencies due to their elevated discharge temperatures which reduce the energy consumption of membrane distillation. In addition, these materials have high volumetric energy storage density, which enables capture and transportation of waste heat from remote locations such as natural gas compressor stations to the well sites, yielding up to 70% reduction in transportation costs relative to moving produced water to centralized treatment facilities at natural gas compressor stations. The third chapter of this work demonstrates the importance of selecting appropriate energy storage material for leveraging low-grade thermal energy such as waste heat to power membrane distillation for decentralized wastewater treatment.

With more certainty given in the possibility and logistics of using waste heat for the membrane distillation system in the oil and gas industry, further analysis was needed to evaluate new technologies with existing brine desalination technologies in terms of replacement potential. Four technologies were considered: mechanical vapor compression with a crystallizer, electrodialytic crystallization, membrane distillation with a crystallizer using electrical heating, and membrane distillation with a crystallizer using waste heat. The fourth chapter of this work evaluates the economic and environmental competitiveness of said technologies.

Zero liquid discharge desalination has garnered considerable attention for its potential to mitigate the impact of water scarcity while minimizing environmental consequences associated with ill-managed brine wastes. In the fourth chapter of this work, the economic and environmental competitiveness of an electrodialytic crystallization system designed in recent works was evaluated. It was found that when compared to existing zero liquid discharge technologies, electrodialytic crystallization could compete economically with the potential to reduce costs of zero liquid discharge by over 60% in optimal conditions. However, this high economic competitiveness is not consistent in more conservative operating scenarios. Furthermore, electrodialytic crystallization has 42% lower global warming potential than existing technologies. Scenario and sensitivity assessments completed in this chapter identify the operating parameters of electrodialytic crystallization that greatly affect economic and environmental impacts. Most notably, improvements to the cost and performance of ion exchange membranes will provide the highest benefit to electrodialytic crystallization competitiveness. With appropriate concentration of future research on these high-impact areas, the economic and environmental viability of electrodialytic crystallization should continue to increase in the coming years and electrodialytic crystallization will compete with existing zero liquid discharge technologies to provide a low-cost, efficient, and low-impact replacement to existing technologies. This chapter also shows the limited viability of membrane distillation with a crystallizer in replacing existing zero liquid discharge technologies due to high costs. In either case of electrical heating or waste heat use for membrane distillation, energy costs or infrastructure costs stemming from high energy intensity of membrane distillation result in costs far exceeding those of existing technologies.

Through economic and environmental analysis expand the understanding of the potential for technologies to reach industrial application, further analysis can be leveraged to evaluate the fit of technologies into specific applications based on multiple stakeholder perspectives of the system needs. In the fifth chapter of this work, technology options were qualitatively evaluated under a stakeholder-informed triple bottom line sustainability perspective

Chapter 5 of this work evaluates proposed technical solutions to produced water desalination and considers the additional economic, environmental, and social barriers that exist within the oil and gas industrial system. The consideration of these three impact areas (i.e., economic, environmental, and social) are defined as the triple bottom line considerations. The drivers, pressures, states, impacts and responses framework, first

developed by the European Environmental Agency and later updated by the United States Environmental Protection Agency, was used to support the work of chapter 5 by organizing broad system considerations collected from stakeholder-generated literature into an orderly and approachable list of system indicators to evaluate technology compatibility within the applied system. System indicators are quantified, and overall system compatibility scores are calculated based on a variety of stakeholder preference scenarios. The results show that, given current models, emerging technologies have the potential to compete with existing zero liquid discharge technologies when applied to the oil and gas industry for produced water desalination under applications where stakeholders have low economic preference. Careful consideration of stakeholder preferences is necessary because technologies rank differently based on weightings of economic, environmental, and social impact importance.

In summary, through thermodynamic and system modeling, techno-economic analysis, life cycle assessments, and triple bottom line sustainability considerations, four zero liquid discharge desalination technology options for the oil and gas industry (i.e., mechanical vapor compression with a crystallizer, electrodialytic crystallization, membrane distillation with a crystallizer using electrical heating, and membrane distillation with a crystallizer using waste heat) were evaluated for the Denver-Julesburg Basin in Northern Colorado. Overall, development of ion exchange membranes with improved performance for electrodialytic crystallization and developments in lowering membrane distillation energy intensity will determine the future economic competitiveness of electrodialytic crystallization and membrane distillation, respectively, as desalination technology options over mechanical vapor compression. However, when evaluating triple bottom line sustainability, results show potential for applications where there is lower preference to

economic performance. In such applications, electrodialytic crystallization and membrane distillation with a crystallizer using waste heat consistently compete with mechanical vapor compression-based systems. Further understanding of the applied system needs and stakeholder preferences will determine overall applicability of technologies into the system.

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1. INTRODUCTION AND BACKGROUND

The development of unconventional oil and gas extraction, and particularly the boom in its use, has led to increasing volumes of water being used and wastewaters being produced in the oil and gas industry. Hydraulic fracturing is the most common method of unconventional oil and gas extraction. During hydraulic fracturing, large volumes of water are pumped to a high pressure into fissures throughout the oil and gas formation. This pumping requires a very large amount of energy. During the production phase of the well, oil, natural gas, and water are collected at the surface. Once the oil and natural gas are separated, the collected water (i.e., produced water, PW) is very highly concentrated in salts. PW in some basins reaches 10+ times the salt concentration of seawater [1]. Up to 11 million gallons of fresh water can be used to hydraulicly fracture a single well, which is equal to the yearly consumption of 100 average homes in the U.S. [2]. In 2017, 1.02 trillion gallons of produced water was generated in the US [1]. If all produced water generated were able to offset freshwater use, the U.S. would see roughly a 1% decrease in total freshwater consumption annually [3].

There are multiple regions in the U.S. that produce oil and natural gas (Figure 1). For the sake of exemplifying methodology through application, this work is focused on the Denver-Julesburg Basin in northeastern Colorado (called the Denver Basin in the Figure). In some cases throughout this work, this basin is characterized as Weld County, which is the largest and most productive county within the basin.

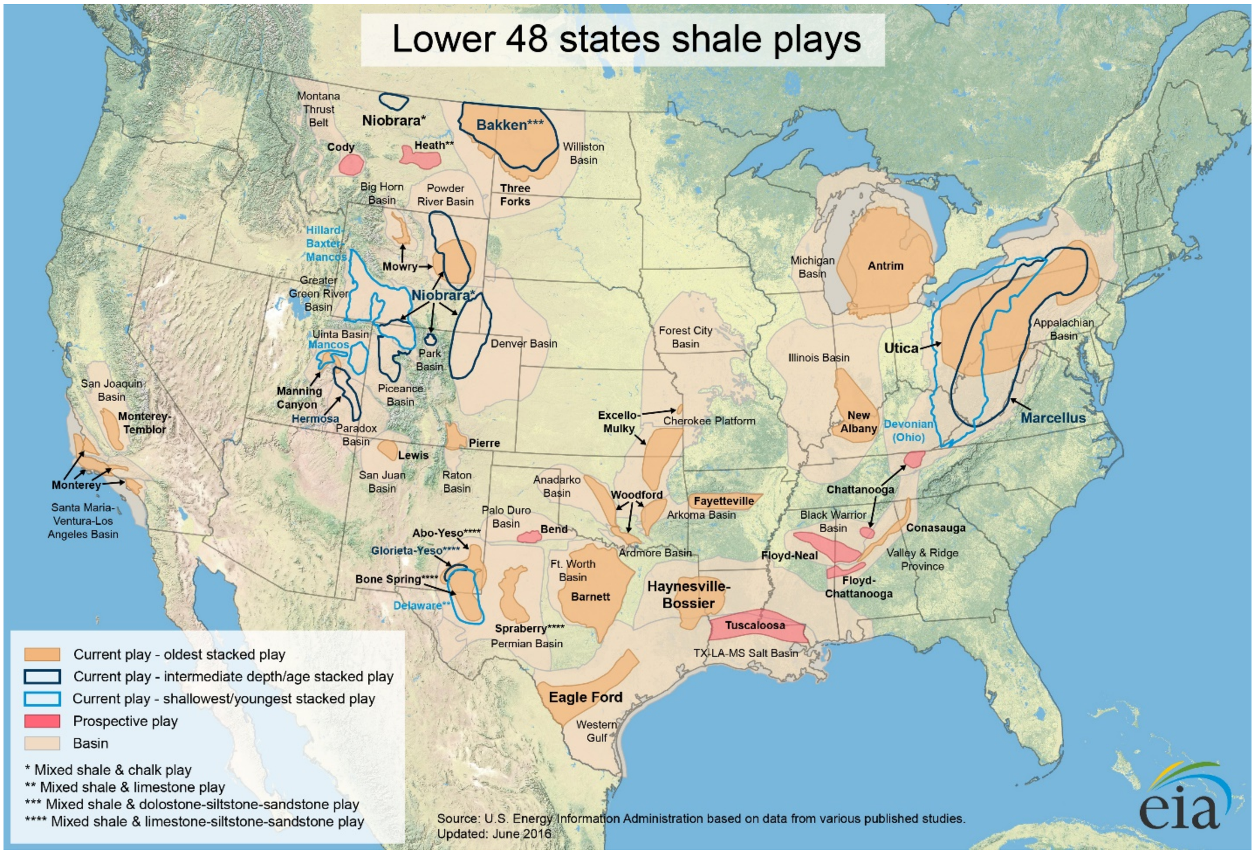

Figure 1: Map of Oil and Gas Producing Locations in the U.S. The Denver-Julesburg Basin, called the Denver Basin in this figure, can be seen in the Northern Colorado, as part of the Niobrara Shale.

1.1. Produced Water in the Denver-Julesburg Basin

1.1.1. Produced Water Volumes and Quality

Weld County generated 2.8 billion gallons of PW in 2020, which is a 769% increase relative to the PW production from 2010 [4]. There were 10,719 wells producing in November of 2022. Robbins et al. studied the flow of produced water in the DJ basin over time, where they noted that during the production phase of a well, up to 40% of production happens in the first year [5]. Even further, produced water volumes are highest within the first 2 months of production. This transience of produced water generation creates more complications in the economics of decentralized treatment systems [6].

The quality of the PW generated in the Denver-Julesburg basin is low, as in all regions of the U.S. However, the concentration of constituents is on the lower end for PW in the nation. Seawater has a total dissolved solids concentration of about 35,000 mg/L. In the DJ Basin, concentrations range from 20,000 to 40,000 mg/L [5]. In other basins, the concentration can exceed 10 times the concentration of seawater, reaching up to 400,000 mg/L [1]. In general, this makes PW desalination in the DJ Basin more attainable than in other regions of the U.S. and makes the DJ Basin a good starting point in the development of PW desalination technologies.

1.1.2. Options for Produced Water Management

Common methods of PW management, which do not change the characteristics of the PW and rather move the PW to another location, were used to handle the PW being generated. The most rudimentary of these methods would be to discharge the water to the surface. Another option was to store PW in evaporation ponds, for natural evaporation of the water to occur. Lastly, deep well injection emerged as a more advanced management method. During injection, class-II injection wells[2] are used to pump the PW back into the ground for long-term, arguably permanent, storage [3]. More active managements (i.e., those that change the state of the PW) methods were not much considered until hydraulic fracturing made its large-scale appearance.

Hydraulic fracturing has increased the volume of PW being used and generated. In the Niobrara Shale, water use per well increased by 146%, from 2.4 million gallons per well in 2011 to 5.9 million gallons per well in 2016 [7]. The drilling lateral length of the average well increased by almost 40%, but the amount of water used per lateral length increased nearly 80% [7]. Management of PW has moved further toward deep well injection. However,

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[2] Class II injection wells are classified by the Environmental Protection Agency, for use by the oil and gas industry for disposal of liquid wastes.

with the larger volumes of water being injected, further externalities are being discovered, such as freshwater contamination and induced seismicity [8-11]. It is also important to mention that the PW being injected takes water away from freshwater cycles, which has especially large impacts in arid regions as in the DJ Basin [1]. These effects of poor PW management have resulted in the examination of active management methods, or treatment.

PW treatment allows for the beneficial reuse of PW and brings water back into the freshwater cycle, either directly or by displacing additional fresh water consumption from within the industry [12]. PW treatment includes multiple steps such as the removal of organics, desalination, and disinfection. This work focuses on desalination of the PW and assumes that all pre and post treatment will be done in similar matters for each technology.

1.2. Produced Water Desalination

1.2.1. Desalination Technologies

Desalination is not a new process, and there are existing technologies such as reverse osmosis which leads the desalination industry [13]. However, existing technologies are limited when applied to PW. As discussed above, PW is a highly saline brine. Reverse osmosis has a limiting salinity of roughly two times the salinity of sea water, or around 70,000 ppm [14]. As such, the mainstream technologies in the desalination industry are not capable of treating PW. There are technologies, such as Mechanical Vapor Compression (MVC), which are designed to operate at higher salinities, but none have shown to be economically competitive or energy efficient enough to transition the PW management industry to treatment.

1.2.2. Desalination Location and Energy Availability

Perhaps the largest question surrounding PW desalination, after what technology to use, is where to install it. Desalination of PW can happen in one of two places: Decentralized, which is at the production well, or centralized, which is at a location where PW from multiple wells can be collected and treated. Decentralized treatment allows for clean water to be produced at the site of oil and gas production. However, it raises problems in energy availability, mobility, and scale. On the other hand, centralized treatment benefits from economies of scale and reliability but requires the transportation of untreated PW from the production well. As PW treatment is still a large area of research, and not a common application within industry, it is not yet known what sort of externalities and impacts may result. The system consideration of PW treatment is important, as when applying any technology for a purpose.

1.3. Organization of This Dissertation

This work is broken into 3 major components. First, and introduction to the system of focus has been provided in this chapter and the following chapter provides a literature review, which evaluated previous work in this area, and lays out the short fallings of existing research. Details on specific aims of this work to fill these gaps can be found in Section 2.3. Chapters 3 through 5 represent three major analyses completed for this work: waste heat utilization for membrane distillation, techno-economic analysis and life cycle assessments, and triple bottom line sustainability, respectively. Third, and lastly, conclusions and recommendations for future work are provided in the last chapter of this work. References and multiple sections of supplementary materials are provided at the end of this document.

2. LITERATURE REVIEW

2.1. Desalination Technologies

Sixty-five percent of desalination technologies applied in the world are reverse osmosis (RO) based systems [13]. Only 2% of applications are using emerging technologies for desalination [13]. It could seem as though RO should be an option for PW desalination. However, because less than 1% of desalination plants are treating brine (i.e., solutions with high salt content), it makes sense that RO has such a large presence [13]. RO is limited in its ability to treat high-salinity brines, with a limiting salinity of approximately 70,000 mg/L [14]. RO, then, is a good technology for desalination of seawater and brackish water, which have salinities up to 35,000 mg/L. Like RO, other membrane-based desalination technologies do not work well when applied to high salinity produced water. Other technologies are being developed to remove higher concentrations of salts from brines [15-23]. Because PW can have salinities up to 400,000 mg/L the following technologies are being studied in literature as options for PW treatment [1].

The technologies developed for brine desalination can be split into two main branches [16, 24-26]. The first branch, thermal desalination, is based theoretically on the direct evaporation of water from non-volatile constituents. On the second branch are hybrid membrane technologies, which operate on thermal and electrical differentials to drive water/constituent flux through a membrane. Table 1 provides the collection of desalination technologies considered in this work, their driving forces, possible energy sources, advantages, and limitations. Each technology is discussed in more detail in the following sections.

Table 1: Produced Water Desalination Technologies. A brief review of mechanical vapor compression, membrane distillation, and electrodialysis, their driving forces, energy source options, and general advantages and limitations.

Technology	Driving Force	Energy Sources	Advantages	Limitations
Mechanical Vapor Compression	• Evaporation	1) Electricity (e.g., compressor) 2) Heat (e.g., pre-heating)	• Energy efficient	• Expensive
Membrane Distillation	• Thermal gradient • Water vapor flux	1) Low Grade Heat 2) High Grade Heat 3) Electricity (e.g., resistive heating)	• Can operate solely on low grade heat	• Low energy efficiency
Electrodialysis	• Electrical gradient • Ion flux	1) Electricity (e.g., voltage supply)	• Energy efficient • No thermal dependance	• Does not produce clean water

Energy sources for desalination include high grade heat, low grade heat, and electricity. In this work, high grade heat is defined as reliably above 100°C. Low grade heat is at or below 100°C. Typically, low grade heat is synonymous with waste heat (WH). Electricity can be converted to other forms of useful energy: electrical, mechanical, or thermal.

During thermal desalination, water is evaporated from non-volatile constituents. The pure water is then re-condensed and collected. Thermal desalination technologies include mechanical vapor compression (MVC, included in this work), multi-effect distillation, and multistage flash desalination [12, 27-30].

The second type of desalination technologies are membrane based. With membranes, there is a necessary driving force to be applied for water or dissolved constituents to travel through the membrane, also called flux. In traditional membrane technologies, like RO, a pressure is applied across a membrane to encourage flux. However, as concentration of constituents increases, necessary pressures increase, resulting in the need for other driving forces as the mechanical limits of membranes are reached [31]. The resultant options for driving forces are thermal and electrical differences. As such, in this work, membrane-based technologies for brine desalination are further described as hybrid membrane technologies.

One each of thermally (i.e., membrane distillation, MD) and electrically (i.e., electrodialysis, ED) driven technologies are considered in this study, though many other variations of hybrid membrane desalination technologies exist [12, 27-30, 32].

Evaporation, or direct boiling, as a thermal desalination technology, requires thermal energy for operation. Furthermore, since water must be essentially boiled out of the brine, a high temperature (i.e., high grade) thermal energy must be provided. This is achievable by using a boiler, which burns a fuel to create direct high grade thermal energy, or with a resistive heater, which consumes electricity to generate a thermal energy source. Low grade thermal energy can still be used in evaporation for preheating of influent brine.

Even though evaporation is not a new or emerging technology in desalination, it is still a useful baseline to compare with other treatment options. First, evaporation is a reliable system for separation of water from dissolved solids. Second, it is theoretically quite simple to model and predict, as the amount of direct thermal energy required for evaporation can be calculated as an enthalpy difference. Lastly, one of the metrics used to compare energy consumption of desalination technologies is based on evaporation, namely gained output ratio (GOR)[3]. However, evaporation is energy intensive, even with systems incorporating thermal energy recovery, and is therefore not a highly considered option for desalination of brines. Evaporation is not considered as a technology option in this work. However, it is important to remember as the baseline for brine desalination energy consumption goals.

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[3] Gained Output Ratio (GOR): A metric used to measure the amount of energy consumed by a desalination process. GOR is the ratio of energy needed for direct evaporation (i.e., without energy recovery) to the amount of energy consumed. For example, a GOR of 1 means that the amount of energy used is equal to the amount of energy needed for evaporation. However, a GOR of 5 would indicate that the amount of energy used is only 20% of the amount of energy needed for evaporation.

2.1.1. Mechanical Vapor Compression

MVC is a high temperature thermal desalination technology, which creates heat for evaporating water by compressing water vapor using an electric compressor, rather than supplying heat through a boiler or resistive heater [33, 34]. There is also energy recovery within MVC that allows for the gained output ratio to exceed 15 [5, 33, 35, 36]. This energy consumption reduction has led to MVC becoming the state art technology for high salinity brine desalination. MVC operates on electricity, which is used in the compressor to raise the pressure of a water vapor flow. However, both high and low grade thermal energy can be used to preheat the brine coming into the system, which reduces the amount of work that must be done by the compressor.

Unfortunately, MVC is not without its problems. The material needed to build the MVC unit that limits deterioration in the high temperature and high salinity environment (i.e., titanium) is expensive [37, 38]. As such, treatment by MVC results in very high capital costs which limit the adoption of the technology. Furthermore, MVC has been shown to be highly sensitive to economies of scale, thus it is not often thought of for treatment of PW [6, 37]. However, MVC may be competitive in centralized PW desalination settings where economies of scale can be taken advantage of [38].

2.1.2. Membrane Distillation

MD is categorized as a hybrid membrane desalination technology. However, water flux through the membrane is driven by a temperature difference across the membrane. A warm brine (~90°C) is flowing on one side of a hydrophobic membrane while on the other side is a cool clean distillate (~40°C) flow [5, 23, 31, 34, 35, 37, 39-47]. The temperature difference across the membrane creates a vapor pressure difference across the membrane.

Water in the warm brine evaporates at the membrane and can travel through the hydrophobic membrane then condense into the cool distillate.

Because MD does not operate at high temperatures, it does not require expensive non-corrosive materials [5, 6, 37, 47]. This lowers the capital expenses associated with MD and makes it economically competitive with MVC. MD, however, is less energy efficient, achieving a GOR of closer to 2 [5, 35]. As energy availability in decentralized locations is already questionable, utilization of higher amounts of energy may limit the adoption of MD in addition to increasing operational costs.

Luckily, MD does not require a very large temperature difference across the membrane to drive water flux and does not depend on high grade thermal energy or electricity to operate. MD is the only technology evaluated that can operate completely from low grade thermal energy but can still use high grade heat or electricity through resistive heating as an energy source.

2.1.3. Electrodialysis and Electrodialytic Crystallization

ED has begun to emerge as a technology for brine desalination [48-56]. Traditionally, ED was used in low-salinity situations because it is only energy efficient with lower salinity differences between the brine and distillate flows. However, a higher salinity brine can be used in a module with a slightly lower salinity, which produces crystalized salt and a slightly desalinated brine [49]. The lower salinity brine can then either be desalinated in a more reliable desalination technology such as RO or with additional ED modules in series. The unique cation and anion exchange membranes of ED allow ions to be driven across by an electrical potential difference across the ED module, which is supplied by electricity. ED is the only technology evaluated that does not require thermal energy for operation. However, this means that the only energy source that can be utilized by ED is electricity. Depending on the energy availability and accessibility for decentralized treatment scenarios, this may be a barrier to implementation.

Electrodialytic Crystallization (EDC) is an adaption to ED, where an ED module concentrates a brine to saturation. The saturated brine is sent to a crystallization tank for solids settlement. The less-concentrated brine produced in the ED module is sent to an RO unit, and re-constituted to the original ED module inlet salinity, while also producing a clean water product. The EDC configuration was proposed by Zhang et al. [57]. In this work, ED is not evaluated independently, and the configuration of EDC is used.

2.1.4. Zero-Liquid Discharge

Desalination of brines is the process of separating water and salts. In some cases, as with RO, technologies remove clean water from a brine and generate a clean water stream and a further concentrated brine stream. Other technologies like ED remove the salt from incoming brine to produce a lower salinity brine and a salt concentrate. The idea of zero liquid discharge (ZLD) desalination is to completely separate water from dry salts.

ZLD has two major advantages. Firstly, all water is removed from the brine, allowing for the maximum possible beneficial reuse of water [12]. Second, waste management becomes easier as the byproduct of desalination becomes dry salt instead of a liquid brine [12]. However, ZLD further increases the size of desalination technologies and subsequently the energy consumption and cost of the systems [12]. To remove the need for deep well injection completely, ZLD is, nevertheless, necessary.

All technologies discussed above, ED, MVC, and MD, require the use of an additional concentrator to achieve ZLD. The MVC and MD technologies each require a crystallizer to achieve ZLD because they produce a clean water and a concentrated brine by-product. The concentrated brine is fed to a crystallizer to remove the remaining water from the dry salts. The combination of these technologies with a crystallizer is denoted as MVC+C and MD+C, respectively. ED also requires additional technologies to achieve ZLD. However, ED does not generate clean water and requires a technology such as RO to produce a clean water product using the lower salinity brine which is produced by ED. The ZLD combination of ED, crystallization tank, and RO technologies have been described in publications as EDC [57].

2.2. Limitations to Produced Water Desalination and Gaps in Research

In general, limitations to PW desalination can be consolidated, no matter the technology, into four major areas: Energy availability and accessibility, financials, environmental impacts, and general sustainability.

2.2.1. Energy Availability & Possible Energy Pathways

After understanding the basics of the technology operational advantages and limitations, thought of broader system design leads to complications in energy availability and accessibility. PW is generated in scattered locations throughout the U.S. Many of these locations are void of industrial development (such as access to electricity). All proposed treatment technologies, inducing the thermal and hybrid membrane systems discussed in this work, require some amount of energy to operate. Some of the technologies (i.e., MD) rely on low-grade thermal energy, which most-abundantly takes the form of waste heat. Not only is there question of how much energy is needed, both at centralized and decentralized locations, but there is also the question of the usefulness of the available energy [5, 6, 38, 44, 46]. As explained above, some technologies can operate with low grade heat, and others demand electricity or high-grade heat. EDC and MVC+C require electricity for operation.

Furthermore, the energy available for utilization at decentralized locations is limited compared to centralized locations. The options and availability of each energy source are discussed in the following paragraphs.

On the site of an oil and gas production well, electricity is not abundantly available. There may be a small generator on site that supplies electricity to auxiliary measurement and monitoring equipment, but the amount of electricity generated is negligible compared to the amount that would be needed for desalination. Some production wells are in areas where access to electrical infrastructure is straight forward (i.e., there are powerlines nearby). On other, more rural, production sites, electrical infrastructure is not readily available. As such, to consider electricity as an energy source in decentralized desalination, one must also consider the economic and environmental impacts of building out the infrastructure to deliver that electricity.

Burning of fuel is a basic way of producing heat. There are two main sources of fuel for a decentralized desalination system [5]. First, fuel could be transported onsite using trucking. The second option would be to burn the fuels that are being generated in conjunction with produced water (i.e., burn the natural gas coming from the ground instead of selling it). The study done by Robbins et al. in 2020 showed when using MD as a treatment technology, roughly 10% of the natural gas being produced during peak PW generation would go toward desalination if used as the fuel source [5]. This high-grade heat could also be used as a preheating option for MVC.

Low-grade thermal energy, or WH, is a product of inefficiencies when operating engines and pumps and other technologies. Extra and unused, or wasted, heat can be collected from coolant loops and exhaust streams of engines and pumps. Usually, 60% of the energy supplied as fuel to an engine leaves as waste heat, and 30% is converted into mechanical power [5]. As such, there are two supplies of waste heat for decentralized waste heat. First, there is waste heat from generators that operate during production phases. The problem, as with the electricity availability, is that not enough waste heat is produced for treatment [5]. The other option for on-site waste heat is from the hydraulic fracturing (HF) process. However, there is no PW generation when waste heat from HF is occurring, and even though there is significant WH available, it may not be accessible for utilization due to that temporal difference between availability and use [5].

The use of waste heat as an energy source has been proposed in multiple instances which include from hydraulic fracturing and natural gas compressor stations [5, 38, 46, 47, 58]. However, these studies considered only the quantity of waste heat available in relation to the energy consumption of MD (i.e., the availability). Not considered, is the accessibility of the waste heat. In other words, they have failed to consider the transfer of the waste heat to use. For example, in the case of waste heat from hydraulic fracturing, the waste heat is not available at the same time as it needs to be used – which creates a need for storage of the waste heat for later use. In the case of waste heat from natural gas compressor stations, there is a spatial disparity between waste heat availability and the production of the produced water – which creates a need for the transportation of either PW or for waste heat. Consideration of transportation of PW has been conducted [46]. However, the option of transporting waste heat has not been considered until this work.

Centralized desalination facilities offer a more reliable source of energy in all cases. There is electricity access within a region, fuels can be reliably and predictably be shipped to centralized locations in bulk, and even waste heat from natural gas compressor stations is available in large quantities for centralized treatment [5, 38, 44, 46, 47]. Centralized treatment requires produced water transportation. Therefore, centralized treatment may be less economically and environmentally competitive with decentralized treatment options. However, compared to the common practice of deep well injection, these transportation impacts may be low, especially in regions with limited disposal well access (e.g., the Marcellus shale) [46].

2.2.2. Economics of Produced Water Desalination

A huge, if not the largest, barrier to PW desalination is the cost of treatment. Technologies that can desalinate these difficult to manage waters are expensive [5, 6, 37, 47, 59, 60]. This is especially the case when compared to industrially adopted desalination technologies (i.e., RO) for brackish and seawater desalination. Furthermore, deep well injection is cheap, so it is very hard to compete with the low costs of existing PW management methods [46, 59]. Careful evaluation of the economic impact desalination will have on the industry and communities surrounding oil and gas extraction is needed to determine the feasibility of adoption.

Under the banner of economic impacts, there are several indicators that can be quantified to determine the performance of a treatment scenario. These include capital costs, investment costs, operational costs, maintenance costs, electricity costs, net present value, payback period, minimum selling price, and others [61]. These indicators are the main results from a techno-economic analysis (TEA) and provide an aggregated display of all the results listed above, excluding the payback period. Methodology of a TEA also account for costs in taxes, loan payments, and time value of money [60].

Many proposals have been made for technologies to desalinate PW to ZLD. Some of these proposals have taken the effort to consider a techno-economic analysis of the technology (Table 2). Other studies have conducted TEA comparisons of the technologies for seawater desalination to ZLD (Table 2) [60]. However, there have still been no techno-economic comparisons done for different ZLD options for PW desalination.

Table 2: Techno-economic Analysis of Water Desalination: A collection of studies characterized by the technologies proposed for use, and components considered in the techno-economic analysis.

Author	Year	Technology	Desalination Type	TEA Completed?	Notes
Campisi et al.	2023	• Reverse Electrodialysis	Produced water	Yes $1.44/m³ treated	[62]
Osipi et al.	2018	• Microfiltration-Reverse Osmosis • Microfiltration-Assisted Reverse Osmosis-Reverse Osmosis • Microfiltration-Mechanical Vapor Compression • Forward Osmosis-Mechanical Vapor Compression	Produced water	Yes $1.25-5.45/ m³ treated	[63] The salinity of produced water was evaluated in a range of 50-120 g/L.
Xu et al.	2008	• Nanofiltration • Ultra-low Pressure Reverse Osmosis	Produced water	Yes $0.24-0.27/m³ produced	[64] 1 million gallon per day capacity
Moore et al.	2018	• Membrane Distillation	Pure water	Yes $85/m³ produced	[65] The system model in this work assumes that salinity has little impact on system costs, and therefore evaluates pure water as the influent of the system.
Karapataki	2012	• Reverse Osmosis • Mechanical Vapor Compression • Crystallizer	Produced water	Yes $2.63-62.5/m³ treated	[66]
Coday et al.	2015	• Forward Osmosis	Produced water	Yes $10.62-25.63/m³	[67]
Edalat et al.	2020	• Reverse Osmosis	Produced water	Yes $1.50-1.60/m³	[68] Inlet salinity is 14 g/L
Schwantes et al.	2018	• Membrane Distillation • Mechanical Vapor Compression	Concentrated brine	Yes $4.79-6.65/m³	[37] Concentrated brine is the effluent of RO, with a salinity of roughly 70 g/L
Tavakkoli et al.	2017	• Membrane Distillation	Produced water	Yes $61-66/m³ treated	[47] Costs are so high due to evaluation in the Marcellus shale, where transportation is for very far distances. Availability of waste heat was assessed, but utilization accessibility was not considered.
This Work	**2024**	**• Membrane Distillation + Crystallizer** **• Electrodialytic Crystallization** **• Mechanical Vapor Compression + Crystallizer**	**Produced Water ZLD**	**Yes**	

2.2.3. Environmental Impacts

There have been concerns over the environmental impacts of oil and gas production for years. More recently, concerns over human health impacts and other social sustainability aspects have emerged [69-71]. In both cases, however, there has been little focus on produced water, and a larger concentration on oil and gas production as a whole.

Some studies have focused on environmental impacts of produced water, but not on desalination [67]. Several studies have considered the environmental impacts of hydraulic fracturing and untreated PW [69, 72]. In addition, considerations of the different energy sources for desalination can have a large influence on the impact to the environment, just as it can largely impact economics.

The most common form of environmental impact assessments is a life-cycle assessment (LCA). LCAs are an advanced form of carbon accounting which consider emissions past greenhouse gasses, and which draw very specific boundaries around systems being evaluated. A study of environmental impacts from desalination recently conducted concluded that the main concern for desalination is the energy usage, rather than waste disposal [73]. Though the manufacture and construction of these facilities have an impact, the emissions per product are very low when compared to the emissions from energy consumption and chemical use [74].

Table 3: Environmental Assessments of Desalination Technologies or Produced Water Management: A collection of studies characterized by the technologies proposed for use in desalination of any brine, or by the impacts considered from produced water management.

Author	Year	Technology	Desalination Type	Notes
Lee et al.	2021	• Reverse Osmosis • Forward Osmosis • Multi-stage Flash • Multi-effect Distillation	Seawater Brackish water	[75]
Ihsanullah et al.	2021	• Multi-stage Flash • Multi-effect Distillation • Reverse Osmosis • Forward Osmosis • Membrane Distillation • Electrodialysis • Electrodialysis Reversal	Seawater	[76]
Semiat et al.	2012	• Reverse Osmosis • Electrodialysis • Multi-stage Flash • Multi-effect Distillation • Vapor Compression	Seawater	[77]
Ahmadi et al.	2020	• None Specified	Any	[78]
This Work	**2024**	• **Membrane Distillation + Crystallizer** • **Electrodialytic Crystallization** • **Mechanical Vapor Compression + Crystallizer**	**Produced Water ZLD**	

2.2.4. Social Sustainability

The success of wastewater treatment technologies relies on the balance of environmental, financial, and social factors [73]. Social sustainability is an emerging field compared to economic and environmental assessments. Also, methodology in evaluating social sustainability is much less straight forward. There are many indicators of social sustainability including job opportunities, human health, social acceptability, access to clean water, civic engagement and involvement, worker welfare, equitable allocation, trust, and security, and many more [79-82]. Social considerations in PW management have been largely avoided and need to be addressed independently of oil and gas development in general [83].

This work will not attempt to address social sustainability but will try to understand different stakeholder perspectives surrounding produced water management. This work will also frame produced water desalination systems in terms of a limited triple bottom line sustainability, which includes all three of economic, environmental, and social considerations of sustainability.

2.3. Aims of This Work

Previous research, as discussed in Section 2.2, fails to capture the bigger picture of produced water management through desalination. There have been many studies that have led to progress in the understanding of individual components to the system. However, there is little to no understanding of how implementing desalination of produced water will impact, and be impacted by, the broader system of oil and natural gas extraction. For example, previous research does not determine the feasibility of operating desalination technologies in decentralized treatment due to unknown energy accessibility. Furthermore, there have been no environmental and social sustainability considerations of produced water treatment. Lastly, no studies have defined sustainability of produced water treatment systems (i.e., the combination of technical feasibility with economic, environmental, and social considerations). This work will attempt to address these gaps in 5 major stages. The specific aims of this work are defined as follows:

1) **Characterize the performance of each of the four proposed desalination technologies.** Understanding the way that each proposed desalination technology operates is crucial in determining impacts of their operations. These technology models will be directly used in this work. By having technical models that determine system performance (e.g., energy consumption, size, etc.) from given input parameters (e.g., treatment rate, inlet salinity, etc.), it will be easier to determine the impacts of changing system conditions.

2) **Determine viability of waste heat utilization as an energy source for decentralized produced water desalination.** The availability of electricity for produced water desalination is determined by the proximity to electrical infrastructure. If there is no access to infrastructure, the impacts of building that necessary infrastructure must be determined. Because high-grade heat is generated by burning fuels, impacts of using high-grade heat are determined by the necessary transportation of fuel to the treatment location. Waste heat, on the other hand, needs further considerations for determining its availability and accessibility. The completion of the following 3 tasks (done in Chapter 3 of this work) will determine the viability of using waste heat as an energy source.

   - **Quantify waste heat availability**

     The first step in determining if waste heat can be used is the quantification of waste heat available in both decentralized and centralized locations. Determining the operating systems present in each location, and quantifying the amount of waste heat produced by each, will determine how much produced water can be treated.

   - **Determine storage system operation**

     As discussed in Section 2.2.1, there are both spatial and temporal disparities between waste heat production and utilization phases. As such, for waste heat to be useful, a waste heat storage system must be developed and analyzed. Designing and modelling the operation of this storage system is crucial in evaluating the feasibility of waste heat use.

- **Evaluate system integration with membrane distillation**

  Membrane distillation is the only technology being evaluated which could operate explicitly from waste heat. Membrane distillation is the best technology to pair with waste heat utilization analysis because it will determine the potential of waste heat use in the highest restrictions. Therefore, the final step in determining the possible use of waste heat for produced water desalination is to model waste heat collection, storage and use by membrane distillation in individual scenarios.

3) **Conduct a comparative techno-economic analysis (TEA) of the four proposed desalination technologies.** Determining the cost of each technology will not only feed into Stage 5 of this work but will also allow for direct comparison of technology costs. These three tasks are completed in Chapter 4 of work:

   - **Determine cost of desalination technologies**

     The capital and operational costs of building and operating each technology can be determined based on their technical models and existing technology cost models.

   - **Analyze systems in TEA with discounted cashflow rate of return (DCFROR)**

     The treatment technology cost can then be evaluated through a DCFROR framework, which will return the levelized cost of produced water treatment (i.e., the cost to treat a given volume of produced water), and the lifetime costs of the treatment system.

- **Determine sensitivity of system costs**

  As conditions of the technology operation change (e.g., system size), the cost of the system and levelized costs of treatment change. It is important to consider how these operating parameters affect cost results and by how much.

4) **Calculate environmental impact of the four desalination technologies.** As with the evaluating of economic impacts, calculation of environmental impacts can be done. These analyses are used in Stage 5 and can also be directly compared for each treatment system. The following tasks are completed in Chapter 4:

   - **Determine emissions of desalination technologies**

     The environmental emissions from operating each technology can be determined based on their technical models.

   - **Analyze 3 proposed desalination technologies in a life-cycle assessment (LCA)**

     By taking emissions created from each operation of the desalination technologies, lifetime emissions can be accounted for. Using the LCA methodology will allow for greenhouse gas impacts, in addition to other emissions impacts, to be calculated on both a total and levelized basis for each technology.

   - **Determine sensitivity of system emissions**

     Just as with costs, as conditions of the technology operation change (e.g., system size), the emissions of the system change. It is important to consider how these operating parameters affect emission results and by how much.

5) **Frame produced water management under triple bottom line sustainability.** Framing the system of produced water management in triple bottom line sustainability will help determine the barriers and complications to implementation of new technologies. Additionally, different stakeholders in the area can have vastly different concerns and goals, which are not addressed. Furthermore, by determining sustainability tradeoffs in the system, potential areas important to focus research and improvements on can be identified. The following tasks are completed in Chapter 5 of this work:

   - **Evaluate system through the Drivers, Pressures, States, Impacts, Responses (DPSIR) framework**

     The DPSIR framework is a method of systems thinking which allows the user to determine the broad impacts on and impacts of a system. Using the DPSIR in this work will allow for the identification of impacts that may be missed with only the previously mentioned methods.

   - **Distill important areas of interest from different stakeholder groups**

     By collecting written works from different stakeholder groups and evaluating them for word frequency and word clustering, it may be analyzed what areas each stakeholder finds most important. By comparing these different stakeholder perspectives, more light can be brought upon this complex problem.

   - **Identify sustainability trade-offs**

     Identification of tradeoffs in the treatment systems can be very useful in both the design of new systems and deciding which systems to implement. In this stage, trade-offs could exist within technologies amongst their economic, environmental, and social sustainability indicators. By shifting the importance set upon each of these categories, tradeoffs may exist for technologies, which make treatment decisions ambiguous without further analysis. Identifying these trade-offs allows further, targeted, research to be completed.

This work aims at understanding the broader system of PW desalination and creating a methodology for ranking desalination systems quantitatively to assist in produced water management decision making. The creation of this methodology will, hopefully, lead to an increase in the number of produced water desalination applications. By including an analysis on the performance of different desalination and zero-liquid discharge technologies, consideration of energy availability and accessibility, and assessment of economic, environmental, and social sustainability, a larger understanding of the system is available. The Denver-Julesburg basin will be used as an example location for applying the tools throughout this work.

3. VIABILITY OF WASTE HEAT CAPTURE, STORAGE, AND TRANSPORTATION FOR DECENTRALIZED FLOWBACK AND PRODUCED WATER TREATMENT[4]

3.1. Introduction

As discussed earlier, the energy availability has no significance if access to that energy is not possible. For example, there could be millions of kJ of energy available as waste heat, but that energy is not useful/assessable to ED. In another example, waste heat from natural gas compressor stations is not accessible for decentralized desalination. In one more example, waste heat from hydraulic fracturing is not available for flowback and produced water FPW[5] treatment because the waste heat is only available before FPW is generated.

This chapter addresses these last 2 accessibility issues and assesses the application of waste heat storage and transportation for increasing the accessibility of these energy sources. A wide range of sensible, phase-change, and thermo-chemical storage materials are assessed for their effectiveness at the utilization of waste heat from on-site hydraulic fracturing engines and natural gas compressor stations, to overcome the temporal or spatial mismatch between waste heat availability and FPW generation. Results show that the type of storage material being used can have a high impact on the efficiency of waste heat

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[4] [84] B. M. Grauberger, G. M. Cole, C. A. Robbins, J. C. Quinn, T. Tong, and T. M. Bandhauer, "Viability of waste heat capture, storage, and transportation for decentralized flowback and produced water treatment," *Applied Energy,* vol. 330, p. 120342, 2023/01/15/ 2023, doi: https://doi.org/10.1016/j.apenergy.2022.120342.

[5] FPW, in this chapter, specifically names both flowback and produced water. All other portions of this document reference produced water (PW). PW is meant to approximate FPW, and these nomenclature differences are only due to collaborator preferences from each chapter.

utilization and the treatment capacity of membrane distillation. Sensible storage materials only utilize sensible heat capacities, while phase-change materials have improved performance because they are able to additionally store latent heat. However, sensible and phase-change storage materials lose 11-83% of heat due to conversion inefficiencies caused by their changing temperatures. Thermo-chemical materials, on the other hand, have the highest potential for use because they collect and release heat at constant temperatures. Three thermo-chemical storage materials (magnesium sulfate, magnesium chloride, and calcium sulfate) were identified with the best efficiencies due to their elevated discharge temperatures which reduce the energy consumption of membrane distillation. In addition, these materials have high volumetric energy storage density, which enables capture and transportation of waste heat from remote locations such as natural gas compressor stations to the well sites, yielding up to 70% reduction in transportation costs relative to moving FPW to centralized treatment facilities at natural gas compressor stations. This work, for the first time, demonstrates the importance of selecting appropriate energy storage material for leveraging low-grade thermal energy such as waste heat to power membrane distillation for decentralized wastewater treatment.

The consideration of waste heat storage and the relevant storage materials to overcome the temporal and spatial inconsistencies of the waste heat utilization is an interesting and necessary concept to further address in the analysis of waste heat utilization for membrane distillation powered by waste heat. When evaluating thermal storage materials, a major concern is the heat loss, which can occur for the following reasons. The first reason relates to the transfer of stored heat to surroundings at lower temperatures. Second, once the temperature of the storage materials decreases below the operating temperature of the treatment technology (i.e., MD in the current study), any additional stored heat is unusable. The difference between the initial temperature of the storage materials and the required temperature for treatment needs to be considered. Due to this temperature gap, a portion of the collected waste heat is used to heat the thermal storage material to the minimum operating temperature, rather than being used for treatment. As a result, using waste heat as an energy source may not be as easy as previous studies have assumed [5, 38, 41, 44, 46]. The effects of waste heat storage on waste heat utilization and the efficiency of membrane distillation treatment are underexplored in the literature.

Herein, this chapter investigates the viability of leveraging waste heat for decentralized FPW treatment using membrane distillation by performing systematic assessments through thermodynamic modelling of three waste heat utilization scenarios (Figure 2). In the first scenario, the storage of on-site waste heat for FPW treatment and focus on the temporal disparities between waste heat availability and FPW production is evaluated. Three types of waste heat storage materials (i.e., sensible, phase-change (latent), and thermo-chemical storage materials) are considered in this scenario due to their different properties and behaviors in heat storage and release. The performance of these materials is compared by evaluating the long-term energy consumption of membrane distillation with a new metric, namely apparent specific energy consumption (ASEC) that objectively captures the potential of stored waste heat for FPW treatment. The second scenario proposes a novel approach of transporting waste heat from centralized, consistent sources such as natural gas compressor stations to the well pads for on-site treatment. This strategy avoids temporal mismatches associated with waste heat usage but is subject to spatial mismatches that require the consideration of transportation cost. The economic prospect of this approach is compared with the transportation of FPW to natural gas compressor stations for centralized treatment (i.e., the third scenario). The resultant comparison is determined by the treatment potential of the waste heat storage material (i.e., the volume of treated FPW per volume of fully charged storage material).

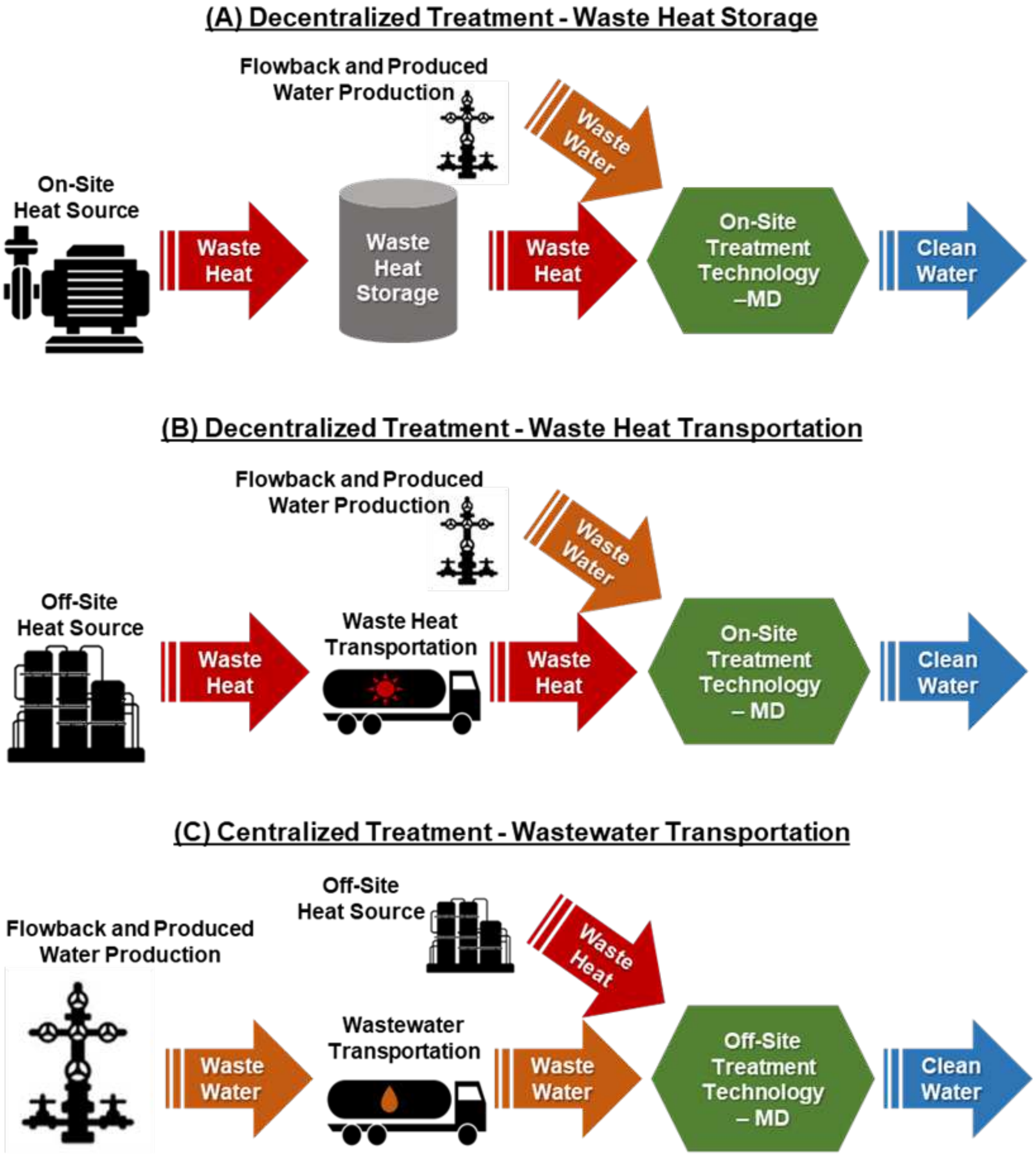

Figure 2: Options of decentralized and centralized flowback and produced water treatment using waste heat from hydraulic fracturing processes as the on-site heat source and waste heat from natural gas compressor stations as the off-site heat source. A) Decentralized treatment using stored waste heat from hydraulic fracturing. B) Decentralized treatment using stored waste heat transported from natural gas compressor stations. C) Centralized treatment of transported flowback and produced water using waste heat at natural gas compressor stations.

3.2. Methods

3.2.1. Waste Heat Availability

The availability of on-site thermal energy sources (i.e., natural gas and waste heat from hydraulic fracturing or on-site generators) was quantified by Robbins et al. [5]. The methodology used in this chapter was duplicated from Robbins et al. to quantify the waste heat available from off-site natural gas compressor stations in the Denver-Julesburg (DJ) Basin.

There are a variety of potential thermal energy sources available during and after hydraulic fracturing (HF) of a well. Potential on-site energy sources include waste heat and well-pad natural gas [85]. Three major sources of waste heat are identified during the lifetime of oil and gas production including the engines and pumps used for HF (pre-production phase), compressors for natural gas pipelines (post-production phase), and engines that provide the full-time electrical energy load required for well site equipment (production phase) (Figure S1, Supporting Information). Alternatively, heat generated from direct burning of natural gas using a boiler paired with a heat exchanger to heat the feedwater could provide the thermal energy necessary for the PW desalination.

The first source of waste heat is from the coolant and exhaust systems of engines and pumps used in the HF process, which produce waste heat for 2-5 days [86-88]. The amount of waste heat was quantitatively estimated at the well sites based on theoretical HF pressures, volumetric flow rate of water used for HF at each well, and component efficiencies. The values of key parameters to calculate available waste heat are detailed in Table S1 of the Supporting Information.

The second source of waste heat is from natural gas compressor stations [38]. While these stations produce a large amount of waste heat, they are not installed at the oil and gas producing sites but rather along the transmission pipelines. Mobile wellhead compression, which is much smaller in size than natural gas compressor stations, may be installed on the well pad but not until the natural gas return pressure drops considerably (typically years after the initial HF of the well) [89]. As a result, such waste heat is not appropriate for on-site wastewater treatment (in particular, during the peak period of wastewater production) and is thus not evaluated further in our study.

The third source of waste heat energy comes from the full-time electrical energy load to operate well site components. In the State of Colorado, the typical configuration for a producing well pad includes wellheads, separation units, tanks, pumps, combustors, air compressors and a remote telemetry unit near the above-ground equipment [90]. The well pad equipment typically only draws a power load of ~8 kW [85, 91]. Details for calculating the waste heat available from producing this amount of electricity with a natural gas or diesel engine is found in Table S2 and Table S3 of the Supporting Information. The thermal energy available from waste heat generated (E_{waste}) due to the on-site electrical loads is a function of the waste heat rate available ($\dot{Q}_{\text{waste}}$) and total operating time (Δt).

$$E_{waste} = \dot{Q}_{waste}\Delta t \tag{1}$$

Further, the energy obtained from burning natural gas (E_{gas}) is a function of the lower heating value (LHV) and the amount of natural gas flow (m_{gas}).

$$E_{gas} = LHV * m_{gas} \tag{2}$$

The LHV of natural gas is based on its composition. The natural gas composition varies by region widely, so care was taken to select a representative composition for the DJ Basin. Based on the U.S. Geological Survey report on unconventional reservoirs in the DJ Basin [92], the composition of natural gas selected for this study was 82.6% methane, 10.1% ethane, 2.7% propane, 0.3% pentane and 2.6% carbon dioxide, with 1.7% of the composition not reported due to the low contents of the remaining compounds. As shown in the Supporting Information, the known parts were normalized to 100% to account for this unknown part of the natural gas composition. By weighting the LHV values of each component, an overall LHV was calculated, and the detailed calculation process is described in Table S4 and Table S5 of the Supporting Information.

3.2.2. Selection of Representative Wells

Methods for selection of the 20 representative wells in the DJ Basin for the following analysis can be found in the publication [84]. This work mainly discusses the results of three wells that represent three general scenarios of utilizing waste heat for FPW treatment. For the first well (i.e., the Varra well), the ratio of available waste heat to FPW treatment demand is low, representing a conservative scenario in which waste heat is likely insufficient to treat all the FPW. For the second well (i.e., the Jaguar well), the ratio of waste heat to FPW is average and represents the average treatment scenario. For the third well (i.e., the Peterson well), there is a high ratio of waste heat available to FPW treatment demand, representing an optimistic scenario in which waste heat is likely more than sufficient to treat all the FPW. As shown in Figure S2B, the three wells we select exhibit the high-end (13.3), average (2.0), and low-end (0.8) of the minimum GOR, at the Varra, Jaguar, and Peterson wells, respectively.

The results of the other 17 wells are presented in the Supporting Information but are not shared in this main text.

3.2.3. Selection of Waste Heat Storage Materials

The selection of waste heat storage materials can be found in the publication [84]. The list of wells and storage materials selected can be found in the Supporting Information. Table S7and Table S8 provide data on the thermal storage materials selected. Visualization of the impact that each thermal storage material can have on storage and utilization of waste heat are provided in Figure 3. All sensible storage materials (SSMs) and phase change materials (PCMs) start at an initial storage temperature (typically ambient temperature), which is assumed to be 20°C in this study. Energy storage in SSMs increase linearly as more heat is added until the temperature reaches the heat source temperature. As heat is removed from SSMs, their temperatures will decrease linearly until reaching the minimum operating temperature of membrane distillation (40°C or 60°C, defined as the critical operating temperature).

Similarly, PCMs also have a linear relationship between temperature and energy content at the beginning of energy storage, but once their phase transition temperature (T_{pc}) is reached, the temperature of the storage material remains constant while energy is added or removed. The amount of energy that can be removed in this constant temperature range is the latent heat. After the phase change process completes, the linear relationship between energy stored and temperature continues. PCMs are heated to the heat source temperature during charging and cooled to the critical operating temperature during discharge.

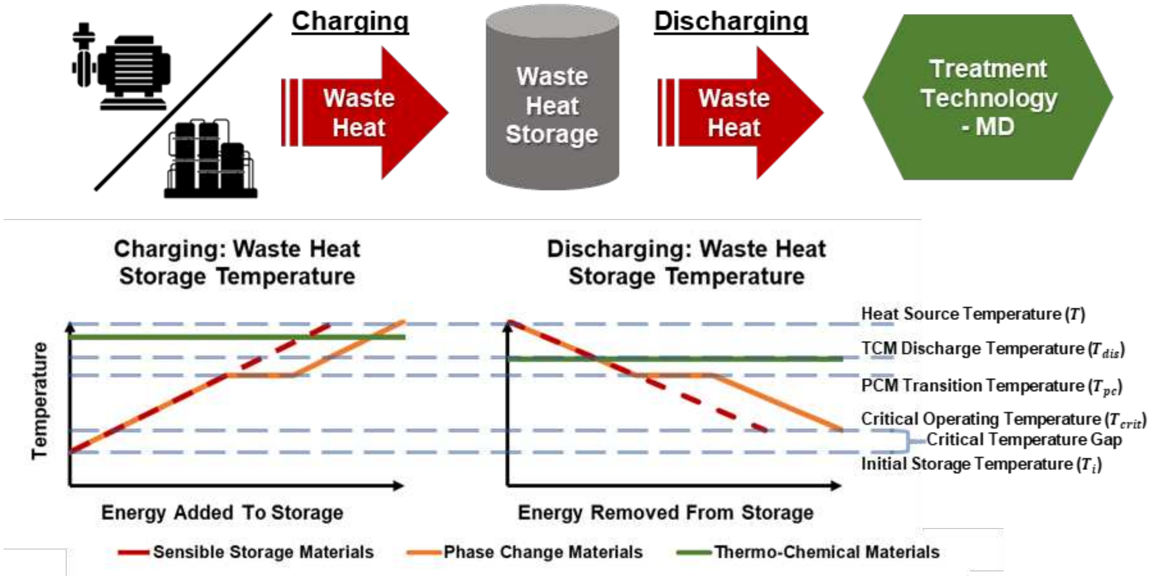

Figure 3: Temperature variance of storage materials given waste heat source temperature, initial temperature of storage material, and critical operating temperature of membrane distillation for a sensible storage material (red), phase change storage material (orange), and thermo-chemical storage material (green).

Sorption allows thermo-chemical storage materials (TCMs) to be charged (desorbed) by a high temperature (T_{charge}) dry flow, which removes the sorbate from the host material. The energy potential of the host material will stay high so long as it is not exposed to the sorbate (water). To recover the stored energy, water vapor is introduced to the sorbent, which ab/adsorbs and releases energy at the desired temperature. This energy is rejected to a fluid that collects the heat released at the temperature used for membrane distillation (T_{dis}). Although this temperature can drop over time, it is assumed for this study that TCMs discharge to the fluid at a constant temperature, which is chosen conservatively [93-99]. This could be an advantage if the discharge temperature is high, but the overall performance could be hindered if the discharge temperature is low. This consideration will be discussed further in Section 3.2.4.

To capture the effect of the critical operating temperature (i.e., the minimum temperature for MD operation) on waste heat utilization viability, the critical operating temperature is assumed to be either 40°C or 60°C in this study. As the critical operating temperature increases, the amount of heat that can be removed from the storage material decreases. Therefore, higher critical operating temperatures decrease waste heat utilization. Moreover, the critical operating temperature directly determines the critical temperature gap, which is the difference between initial storage material temperature and the critical operating temperature. As the critical temperature gap increases, the amount of heat added to the storage material which cannot be used for FPW treatment increases. The impact of the critical temperature gap is higher in SSMs than PCMs and non-existent for TCMs. However, a lower critical operating temperature results in operation of thermally driven treatment technologies at lower energy efficiencies [5, 35, 41]. TCMs are not affected by the critical temperature gap because the temperature of TCMs does not determine the temperature of the fluid charging and discharging the material and as a result, the fluid is assumed to remain at a constant temperature.

3.2.4. *Impact of Waste Heat Temperature on Membrane Distillation Treatment Performance*

It is known that for membrane distillation treatment, the temperature of the heat source (T) (assuming a constant permeate temperature) affects the specific energy consumption (SEC), distillate production rate ($\dot{m}_{clean}$), and feedwater treatment rate ($\dot{V}_{treat}$) [5, 31, 35, 39, 43]. To evaluate the performance of MD modules, the model of MD developed by Robbins et al. was used to provide a relationship between these parameters [5, 44]. For a feedwater temperature ranging from 40 to 90°C, SEC (i.e., the amount of energy used per kilogram of clean water produced) values ranged from 4,369 to 940 kJ/kg (Table

S9, Supporting Information), which are consistent with the values reported in the literature [30, 42, 44, 45].

As energy is extracted from the stored waste heat, the temperature of the storage material can decrease. Consequently, the FPW treatment efficiency of membrane distillation will decrease with time as the storage temperature drops. Steady state performance of MD can be characterized by SEC, which yields the amount of energy used per unit of distillate produced at a fixed temperature. However, because waste heat extraction causes the heat source delivery temperature to change, energy required to drive the MD process changes. The apparent SEC (ASEC) accounts for the waste heat delivery temperature change with time by determining the total amount of energy utilized (WH_{util}) to produce distillate over the full operation lifetime of the treatment technology (FPW_{clean}; Eq. 3).

$$ASEC = \frac{WH_{util}}{FPW_{clean}} \tag{3}$$

3.2.5. Modelling of Waste Heat Utilization and Storage

There are two distinct steps in modelling waste heat utilization: the charging and the discharging phases. During the charging phase, waste heat is collected from a source (e.g., the hydraulic fracturing process) and added to the storage material. During the discharging phase, heat is removed from the storage material to power MD for FPW treatment. Each phase is discussed in the following sections.

3.2.5.1. Charging Storage Materials with Collected Waste Heat

The number of membrane distillation modules used at a given well (N), mass of the storage materials (m_{store}), and volume of the storage material (V_{store}) were calculated at the beginning of each system model. Multiple MD modules are needed for treatment because of the limited treatment capacity of a single MD module. To ensure a reasonable comparison between wells, the number of MD modules is only dependent on the FPW production rate at a well (FPW_{day}; Table S6) and the maximum FPW treatment rate of a single MD module (i.e., $\dot{V}_{\text{treat}}$ at the maximum feedwater temperature; Table S6; Eq. 4). The calculation is rounded up to the nearest number of full modules. With N modules at the well and a sufficiently high temperature heat source, membrane distillation could potentially treat all FPW at the well.

$$N = roundup\left(\frac{FPW_{day}}{max(\dot{V}_{treat})}\right) \tag{4}$$

The mass and volume of storage materials needed to capture the waste heat from hydraulic fracturing (WH; Table S6) are unique to the well and waste heat storage material (Eqs. 5 and 6). Properties of each material can be found in Table S7 and Table S8. For SSMs and PCMs, the change in enthalpy from ambient to maximum membrane distillation temperature (ΔH) determined the required mass of the storage material. ΔH is equal to the difference between enthalpies (h) for the material at its initial temperature (T_i) before charging and the temperature of the heat source (Eq. 5.2). In this case, the temperature of the heat source is assumed to be 90°C for SSMs and PCMs and is identical to the high temperature limit for operation of MD (T_{high}). Because neither charge nor discharge performance of the TCMs depend on mass, the mass of this storage material is not needed or calculated.

$$m_{store} = \frac{WH}{\Delta H} \tag{5.1}$$

$$\Delta H = h(T_{high}) - h(T_i) \tag{5.2}$$

The energy density (E_{density}) of the thermal storage materials was used to determine the needed volume of storage material (Eq. 6.1). For SSMs and PCMs, E_{density} is identical to the change in enthalpy from T_i to T_{high} multiplied by the density of the material (ρ; Eq. 6.2). Because there is no temperature change within TCMs, the same method cannot be used for calculating energy density. For TCMs, the energy density is a value given in the literature based on the potential for reactions within a representatively designed system. These values are recorded in Table S8.

$$V_{store} = \frac{WH}{E_{density}} \tag{6.1}$$

$$E_{density} = \Delta H * \rho \tag{6.2}$$

Alternatively, volume of the storage material can be calculated by dividing the mass of the storage material by the material density. An example calculation for the charging model is done for each storage material type in Table S10 (in the Supporting Information) for the Jaguar well. Comparison of the needed volume of storage material shows that the energy density of a material has a significant effect on the volume of storage material. The volume of the storage material is important because storage tanks are significantly more expensive as they become larger. Therefore, the goal is to maximize energy density so that the storage material volume, as well as the corresponding storage container size, can be minimized.

3.2.5.2. Discharging Storage Materials for Treatment

The steady state operating conditions for membrane distillation in Table S9 were used to calculate treatment system performance as the temperature of the stored waste heat changes. The model considers the system in discretized time portions (Δt) of 0.1 days.

Energy extracted from the stored waste heat was assumed equal to the amount of heat supplied to MD for treatment at a given operating condition. This model tracks the temperature drop of SSMs and PCMs as heat is extracted from the system. The model is run until either the temperature of storage material has dropped to the critical operating temperature of the membrane distillation module ($T_{\mathrm{crit-low}} = 40°\mathrm{C}$ or $T_{\mathrm{crit-high}} = 60°\mathrm{C}$), all the FPW volume was treated, or all the waste heat was used. Two critical operating temperatures were considered to determine its impact on treatment and waste heat utilization. The beginning temperature of the storage material is assumed to be 90°C. TCMs do not change temperature as heat is removed from them, so there is no need for the calculation of new system temperatures. This also means that the system performance will not change over time. Constant performance could be advantageous if the discharge temperature of the system is higher, as efficiency of the system is relatively low at lower discharge temperatures (i.e., more energy will be used to treat FPW, and it will take longer to create similar volumes of distillate).

The amount of energy removed from the thermal storage material at any point in time ($\dot{E}$) is equal to the amount of energy consumed by N membrane distillation modules at the current temperature of the storage material (T) (Eq. 7). Because the energy consumption at any moment is represented with SEC ($SEC(T)$), the distillate production rate ($\dot{m}_{\mathrm{clean}}(T)$) is also calculated from Table S9 to determine energy consumption of the system.

$$\dot{E} = N * SEC(T) * \dot{m}_{clean}(T) \tag{7}$$

There is also a significant amount of heat lost to the atmosphere while in storage ($\dot{Q}_{loss}$). This loss is calculated by assuming a 10-meter-tall tank is used to store the waste heat which is insulated with 5 cm of fiberglass insulation, which has a thermal conductivity of 0.04 $W/m * K$, and a heat transfer coefficient of 10 $W/m^2 * K$ [100, 101]. The diameter of the tank is determined by the necessary volume of the tank, as calculated above (Eq. 6.1). The thermal resistance of the tank walls (Res_{ins}) were determined, and the incremental heat loss was calculated (Eq. 8).

$$\dot{Q}_{loss} = (T - T_i)/Res_{ins} \tag{8}$$

This energy is removed from the thermal storage material, lowering the enthalpy of the remaining material based on Eq. 9.

$$\Delta h = -((\dot{E} + \dot{Q}_{loss}) * \Delta t)/m_{store} \tag{9}$$

With this rate of energy extracted, the new temperature of the storage material (T_{new}) can be calculated based on the amount of energy that has been removed from the storage material. The change in temperature is based on the current temperature of the storage material and the type of material being evaluated. For SSMs, only Eq. 10a is needed because there is no phase change. The change in temperature is equal to the change in enthalpy of the system divided by the specific heat of the storage material (c_p), which is assumed constant within phases. PCMs require the use of conditional functions. Phase change will only occur in PCMs when the temperature of the system is equal to the phase change temperature (T_{pc}). If the current temperature of the system is not equal to the phase change temperature, the system is evaluated using the same methods as for SSMs (Eq. 10a). Once the phase change temperature is reached, heat continues to be removed until the phase change is complete, without changing the temperature (Eq. 10b). Once phase change is completed, the PCM will continue to drop in temperature until the critical operating temperature is reached (Eq. 10a). The liquid fraction (x_{pc}) change is tracked through Eq. 11. The liquid fraction is equal to 1 when the PCM is in the liquid phase, or when its temperature is above the phase change temperature (Eq. 12a). When the temperature of the PCM is below the phase change temperature, the liquid fraction is 0 (Eq. 12b).

$$T_{new} - T = \begin{cases} a)\ \frac{\Delta h}{c_p} & T \neq T_{pc} \\ b)\ 0 & T = T_{pc}\ \ and\ \ 0 < x_{pc} < 1 \end{cases} \tag{10}$$

$$\Delta x_{pc} = \begin{cases} a)\ 0 & T \neq T_{pc} \\ b)\ \frac{\Delta h * m_{store}}{\Delta h_{pc}} & T = T_{pc} \end{cases} \tag{11}$$

$$x_{pc} = \begin{cases} a)\ 1 & T > T_{pc} \\ b)\ 0 & T < T_{pc} \end{cases} \tag{12}$$

Waste heat utilization (WH_{util}) is calculated using Eq. 13. This will return the total amount of waste heat removed from storage for FPW treatment.

$$WH_{util} = \int_0^t \dot{E}\, dt \tag{13}$$

Similarly, the amount of flowback and produced water treated (FPW_{treat}) and the amount of clean water produced (FPW_{clean}) are tracked throughout the model.

$$FPW_{treat} = \int_0^t \dot{V}_{treat}\, dt \tag{14}$$

$$FPW_{clean} = \int_0^t \dot{m}_{clean}\, dt \tag{15}$$

3.2.6. Transport of Off-Site Waste Heat Sources

In addition to the use of waste heat generated on-site from hydraulic fracturing, this study also evaluates the potential of off-site waste heat sources for FPW treatment. The most promising off-site waste heat source has been identified as natural gas compressor stations [5, 38, 44, 46]. These pumping stations are very large and operate continuously. Earlier research on oil and gas production in the DJ Basin has shown that upwards of 70% of natural gas compressor stations would supply sufficient waste heat for FPW treatment after distance optimization [46]. It is also an important consideration that as oil and gas production increases within a specific area, the amount of waste heat from the growing number of natural gas compressor stations will increase and meet rising demands for FPW treatment. Furthermore, the temperature of the waste heat is likewise conservatively approximated as 90°C for SSMs and PCMs.

The challenge in utilization of waste heat from natural gas compressors stations is the spatial disparity between waste heat availability and FPW production. Therefore, either the waste heat must be transported to the well (Figure 2B) or the FPW must be transported to natural gas compressor stations (Figure 2C) for treatment. The number of trucks needed for the transportation of storage material (Eq. 16) and FPW (Eq. 17) were calculated for each storage material and well combination based on a given truck volume (V_{truck}) of 6,000 $gallons$ [102].

$$Trucks\ for\ Storage\ Material\ = max\ (\frac{V_{store}}{V_{truck}}, X_w \frac{V_{store}}{V_{truck}}) \tag{16}$$

$$Trucks\ for\ FPW\ = \frac{FPW_{treat}}{V_{truck}} \tag{17}$$

The potential economic prospects of these two options can be compared on both a volumetric and weight basis. The distance between the well and natural gas compressor station is constant, but the number of trucks needed for transporting FPW and storage material vary. The ratio of storage material volume to the volume of treated FPW is calculated using Equation 18. When this ratio is above 1, it requires more trucks to transport waste heat to a producing well than transporting FPW to a natural gas compressor station. However, this is based only on a volumetric consideration. The additional consideration of weight is needed to determine the actual total number of trucks needed for transportation of waste heat.

$$Volumetric\ Ratio = \frac{V_{store}}{FPW_{treat}} \tag{18}$$

In the scenarios where volumetric treatment capacity of a material allows for transportation of waste heat, the additional step is taken to determine the weight of the material. This is done by determining a multiplication factor (X_w) for each material that transforms the number of trucks needed based on volume to the number of trucks needed based on mass. The methods for determining this multiplication factor are discussed in Section S.3.4 of the Supporting Information. By adding this consideration, we can now calculate the transportation ratio (Eq. 19). When the transportation ratio is below 1, it takes less trucks to transport waste heat to wells than to move FPW to natural gas compressor stations. In such scenarios, the transportation of waste heat to the producing well is economically more favorable by reducing the transportation cost.

$$Transportation\ Ratio = \frac{Trucks\ for\ Storage\ Material}{Trucks\ for\ FPW} \tag{19}$$

3.3. Results

3.3.1. Utilization of Waste Heat for the Treatment of Produced Water

The operation of MD determines the efficiencies of both waste heat utilization and FPW treatment, which are also dependent on the storage materials being used. FPW treatment will stop when the storage material has reached the critical operating temperature, all the FPW has been treated, or all the available waste heat has been consumed. It can be determined which of these criteria is reached first by observing Figure 4, Figure 5, and Figure 6. In these sets of graphs, the fraction of waste heat utilization (top) and fraction of FPW treated (bottom) are tracked along the delivery temperature of stored heat from SSMs (A), PCMs (B), and TCMs (C). The critical operating temperature of 40°C is shown for SSMs and PCMs, which helps determine when treatment is concluded due to insufficient temperatures (e.g., Figure 5A). For the sake of not over-crowding the figures, not all PCMs or TCMs are shown. The materials shown in the main text were selected to show the range of phase change and discharge temperatures of the materials. Results for the other materials can be found in the Supporting Information.

For the Peterson well (i.e., the optimistic scenario for treatment), using water as a thermal storage material did not reach full waste heat utilization nor did the system reach full FPW treatment (Figure 4A). Therefore, the storage system had to have met the critical operating temperature of membrane distillation. Though most of the PCMs near full treatment, only stearic acid achieves full treatment. TCMs are more successful. The only TCM that does not result in full treatment at the Peterson well is lithium bromide which enables 66% treatment (Figure 4C). Because lithium bromide has a very low discharge temperature (close to the critical operating temperature of MD, Table S8), the system operates at low performance in terms of both energy efficiency and treatment capacity.

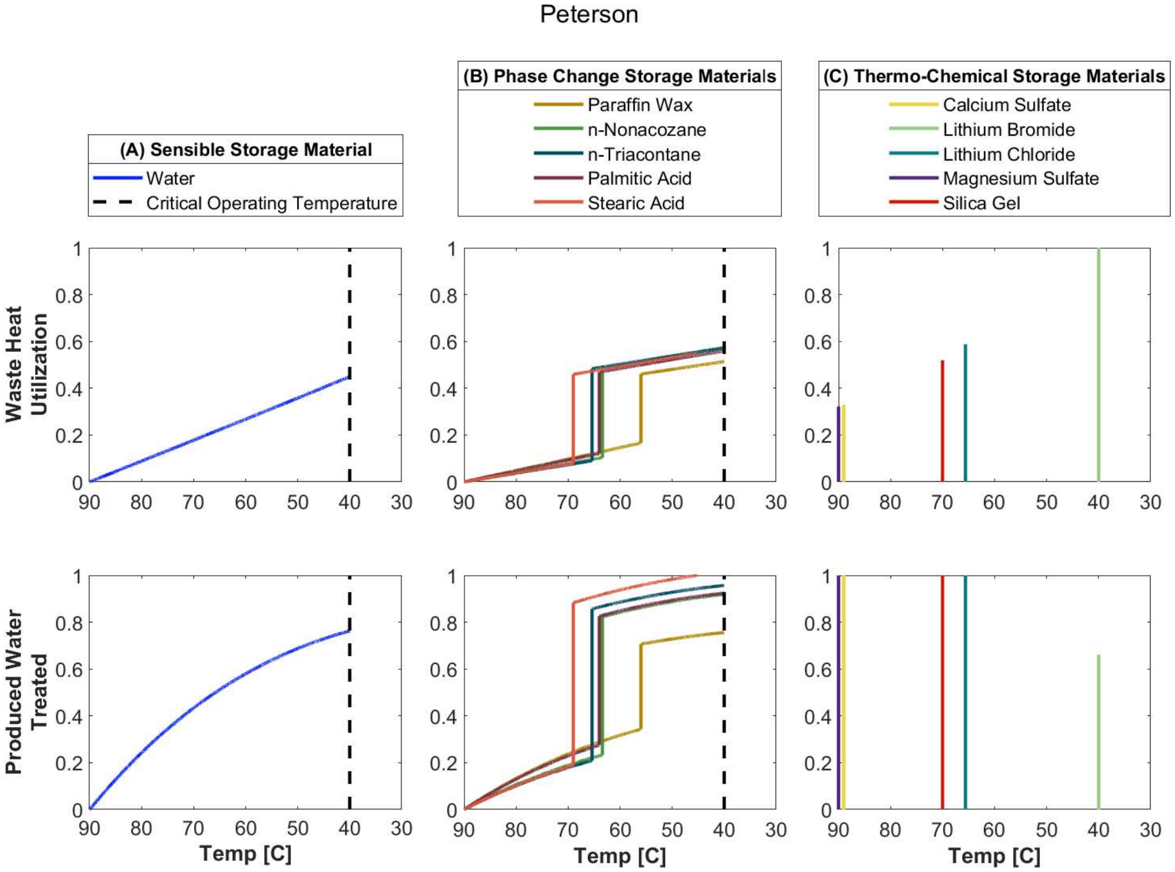

Figure 4: Utilization of waste heat (top) and flowback and produced water treated (bottom) in relation to the storage material temperature for sensible (A), phase-change (B), and thermo-chemical (C) storage materials at the Peterson well, the optimistic treatment scenario. The fraction of waste heat utilization and fraction of flowback and produced water treated are tracked along the delivery temperature of heat from the storage materials.

The Jaguar well, which represents the average scenario, has less favorable results for FPW treatment compared to the optimistic Peterson well. For most storage materials being used at this well, FPW treatment demand is not met (i.e., less than 100% FPW is treated) and waste heat is extracted from the storage material until the critical operating temperature is reached (Figure 5). For example, with a critical operating temperature at 40°C, 37%-50% of FPW is treated when SSM (i.e., water in this study) and PCMs are used, with 60%-75% of waste heat utilized (Figure 5A and Figure 5B). However, when TCMs are used, 86%-100% of waste heat is utilized to treat 25%-100% of FPW (Figure 5C). The materials achieving 100% FPW treatment at this well include magnesium sulfate, magnesium chloride, and calcium sulfate, which are concluded later in this work to be the best options for waste heat storage for FPW treatment. Furthermore, Figure 6 shows results for the conservative scenario (i.e., the Varra well). Due to the high amount of FPW generated at this well, only a small fraction of FPW is treated when the storage materials reach the critical operating temperature, regardless of the materials used for waste heat storage. Therefore, the waste heat generated from hydraulic fracturing on-site is not meeting the treatment demand of FPW in such a scenario.

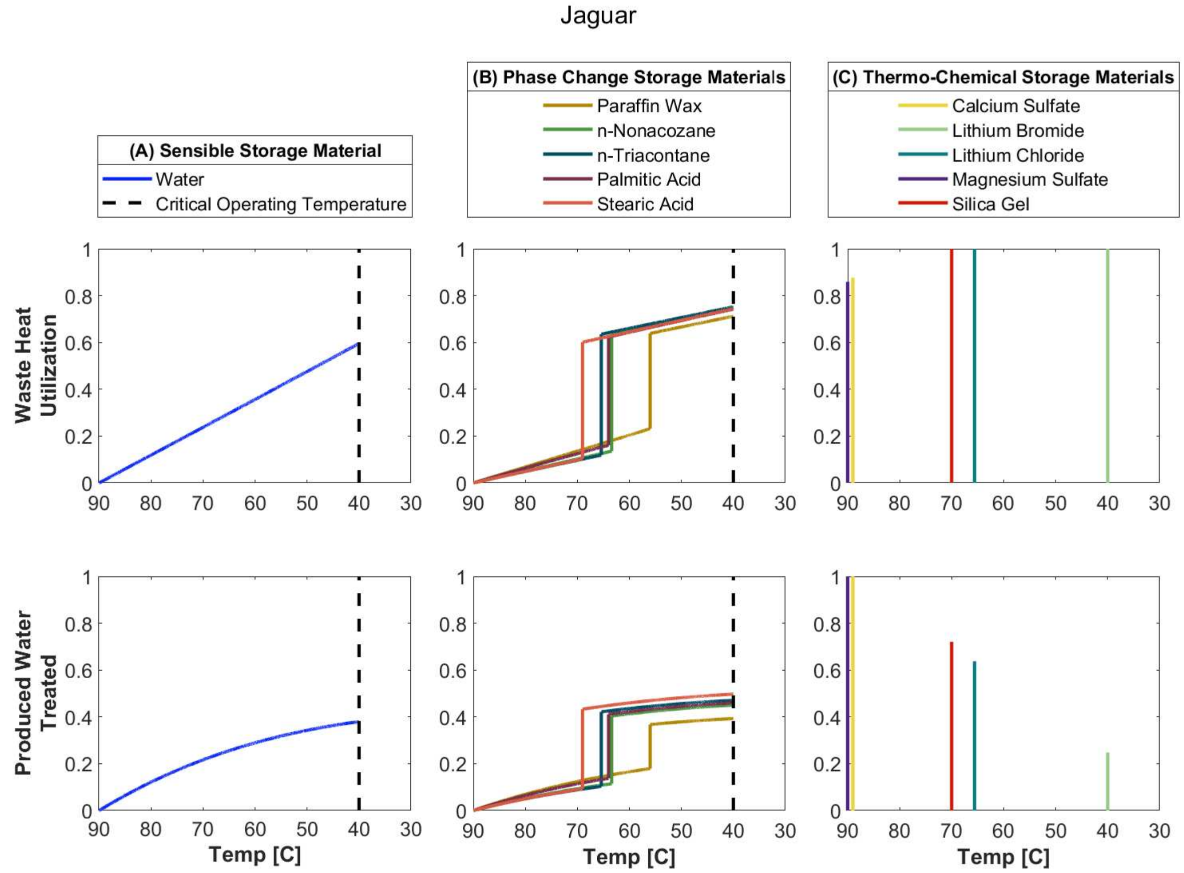

Figure 5: Utilization of waste heat (top) and flowback and produced water treated (bottom) in relation to the storage material temperature for sensible (A), phase-change (B), and thermo-chemical (C) storage materials at the Jaguar well, the average treatment scenario. The fraction of waste heat utilization and fraction of flowback and produced water treated are tracked along the delivery temperature of heat from the storage materials.

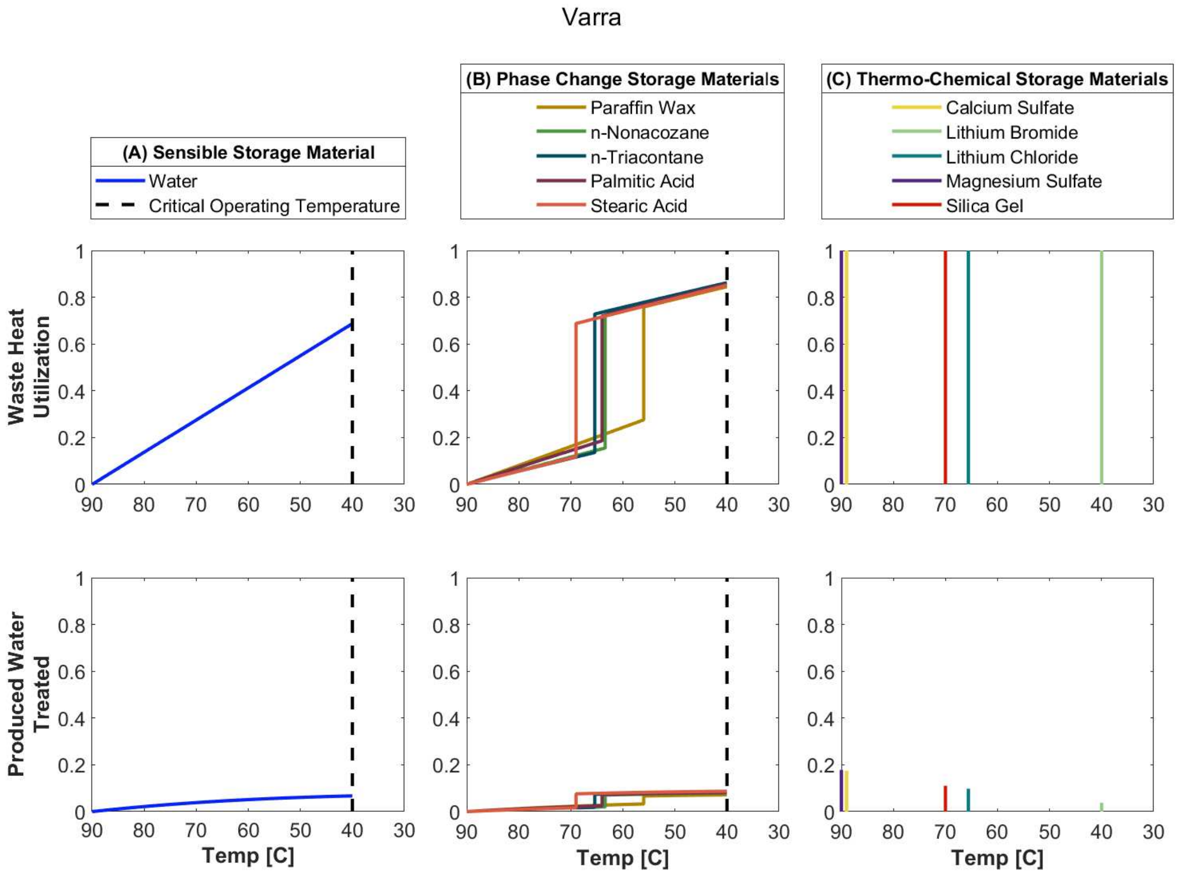

Figure 6: Utilization of waste heat (top) and flowback and produced water treated (bottom) in relation to the storage material temperature for sensible (A), phase-change (B), and thermo-chemical (C) storage materials at the Varra well, the conservative treatment scenario. The fraction of waste heat utilization and fraction of flowback and produced water treated are tracked along the delivery temperature of heat from the storage materials.

Among the 20 wells evaluated by this study, 1 well, Stromberger, experienced 100% treatment of FPW for all storage materials. The Stromberger well performs better than the average levels, thereby representing the optimistic scenario. At 4 wells, 100% FPW treatment is only possible when TCMs with very high discharge temperatures are used (i.e., calcium sulfate, magnesium sulfate, and magnesium chloride). Also, 7 wells have below-average results, where 100% FPW treatment is not possible, no matter which storage material is used. Additionally, 13 wells have results showing that at least one storage material provides possibility for 100% FPW treatment. All the findings above are distilled from the results from the 20 wells investigated in this study (3 wells shown in the main text and 17 wells summarized in the Supporting Information).

The difference among the storage material types for waste heat utilization can be further investigated. The constant decrease in temperature for a SSM is a disadvantage that results in lower performance (i.e., higher energy consumption to produce similar volumes of water) over the treatment period (Figure 5). In contrast, PCMs can take advantage of constant temperatures during heat transfer in latent heat ranges. Even further, TCMs always operate at constant temperature and allows TCMs with high discharge temperatures to outperform both SSMs and PCMs. Using the baseline case at the Jaguar well as an example, the use of water as the storage material allowed the system to treat 38% of FPW when the critical operating temperature is 40°C (Figure 5A). At the same critical operating temperature, the use of PCMs results in 37%-50% of FPW being treated (Figure 5B). By taking advantage of constant temperature during discharge, TCMs are capable of meeting 54-100% treatment demand when excluding lithium bromide (Figure 5C).

The transition temperature of PCMs and the discharge temperature of TCMs play important roles in determining the energy consumption and treatment capacity of MD systems coupled with thermal energy storage. As stated earlier, MD treatment performs better (i.e., with lower energy consumption and higher treatment rates) when the temperature of the waste heat storage material is higher. In the Peterson well, for example, each of the TCMs, excluding lithium bromide, supply heat to treat the full amount of FPW without using the full potential of stored waste heat (Figure 4). Additionally, PCMs result in very close to full treatment. However, the utilization of waste heat increases as the transition temperature of the PCMs or the discharge temperature of the TCMs lowers (Figure 4).

Because each of these scenarios are treating the same amount of FPW, normalized energy consumption of the treatment system increases as the PCM transition temperature or TCM discharge temperature decreases. This relationship arises because materials with a higher transition temperature or discharge temperature can maintain better performance of MD treatment technology (i.e., operate at higher temperatures) for longer periods. Such behaviors will be captured using the new metric (i.e., ASEC) as detailed in the next section.

As clearly shown for the Jaguar well, a higher PCM transition temperature or higher TCM discharge temperature results in a higher FPW treatment capacity by MD (Figure 5B and Figure 5C). For example, the use of stearic acid, which has a transition temperature of 69°C, results in 11% more treatment than the use of paraffin wax, which has a transition temperature of 56°C. Because all PCMs are using roughly the same amount of waste heat, and all TCMs except for calcium sulfate and magnesium sulfate have the same waste heat utilization, it can be concluded that FPW treatment capacity is higher when PCM transition temperatures or TCM discharge temperatures are higher. A closer look at TCMs show that using materials with high discharge temperatures (i.e., 89°C for calcium sulfate) could result in complete FPW treatment as compared to 25% of FPW treatment when using a TCM with lower discharge temperature (i.e., 40°C for lithium bromide). These relationships are not limited to the Jaguar well. Higher PCM transition temperatures and higher TCM discharge temperatures result in higher treatment capacities and lower energy consumption of MD per unit of clean water produced (i.e., having lower ASEC values) for all the wells investigated in this study.

Table 4: Maximum waste heat utilization for all materials given the two different critical operating temperatures

Material	**Maximum WH_{util} (%)**	
	$T_{crit} = 40$°C	$T_{crit} = 60$°C
Water	71	43
Paraffin Wax*	89	26
n-Pentacosane*	89	17
n-Hexacozane*	89	17
n-Heptacozane*	89	17
n-Nonacozane	89	77
n-Triacontane	89	79
Myristic Acid*	87	19
Palmitic Acid	89	77
Stearic Acid	88	77
Calcium Sulfate	100	100
Lithium Bromide*	100	0
Lithium Chloride	100	100
Magnesium Chloride	100	100
Magnesium Sulfate	100	100
Potassium Hydroxide	100	100
Silica Gel	100	100
Sodium Hydroxide	100	100
Zeolite 13X	100	100
Zeolite 13XBF	100	100
Zeolite 4A	100	100

*These accented waste heat storage materials have PCM transition temperatures or TCM discharge temperatures below the higher critical operating temperature of 60°C.

The above analyses show that when waste heat is not sufficient to treat all the FPW (e.g., for the Jaguar and Varra wells), not all the available waste heat could be utilized for treatment using SSMs or PCMs due to the presence of a critical operating temperature. The critical operating temperature, and subsequently the critical temperature gap (Figure 3), drop the maximum waste heat utilization when using waste heat storage materials. As critical temperature gaps become larger, more energy is being dedicated to the pre-heating of the storage material to the critical operating temperature, rather than MD treatment. This energy is lost to the system and removes a portion of the available waste heat for utilization. As a result, each SSM and PCM has a maximum waste heat utilization, which is a property of the system based on both the material being used and the critical operating temperature (Table 4). It is also worth mentioning that the maximum waste heat utilization is a function of MD operational condition and waste heat storage material, but it does not change from well to well.

The transition temperature of PCMs and the discharge temperature of TCMs are also important when considering the critical operating temperature of MD. When the critical operating temperature is higher, some PCMs, with transition temperatures below the critical operating temperature, utilize less waste heat than SSMs (i.e., water) because they are no longer able to store latent heat through phase change and are only leveraging sensible heat (Table 4). For example, at a higher critical operating temperature of 60°C, some PCMs (i.e., paraffin wax, n-pentacosane, n-hexacozane, n-heptacozane, and myristic acid), which have transition temperatures below the critical operating temperature, have low maximum waste heat utilization which ranges from 17-26%, while using water as the storage material achieves a higher waste heat utilization (43%). Meanwhile, the remaining PCMs (i.e., n-nonacozane, n-triacontane, palmitic acid, and stearic acid), which have transition temperatures above the critical operating temperature, result in waste heat utilization ranges from 77-79%. This is another reason that PCMs with higher transition temperatures are of more interest in waste heat storage for flowback and produced water treatment. Furthermore, some TCMs (e.g., lithium bromide) may not be feasible options when higher critical operating temperatures are used, because the discharge temperature is lower than the critical operating temperature. It is worth mentioning that having a lower maximum waste heat utilization does not mean that complete treatment of FPW is impossible. This is especially true in scenarios where there is abundant waste heat available to meet treatment demands.

3.3.2. Apparent Specific Energy Consumption

Although waste heat utilization and treated FPW volumes are important metrics, the ASEC takes both into account and indicates the total treatment system performance when leveraging waste heat to power membrane distillation treatment. This may be the first time a metric accounting for both parameters simultaneously has been used. The ASEC, which is defined as the total amount of waste heat utilized per kilogram of clean water produced, is calculated by generalizing the total energy used and total clean water produced throughout the lifetime of the treatment system (Eq. 3)). The ASEC of membrane distillation when using each storage material was calculated at each well for the range of critical operating temperatures from 40°C to 60°C (Figure 7). As shown in Figure 7, SSMs and PCMs have different ASEC values based on both the critical operating temperature and the well being evaluated. The lowest ASEC value (circle) is associated with the highest critical operating temperature, and the highest ASEC value is indicated by a diamond at the lower critical operating temperature. As the discharge temperature of TCMs does not change as heat is removed, the ASEC value is only dependent on the material type, but not the well. The remaining ASEC data for other wells can be found in the Supporting Information (Table S12-Table S31).

In general, the ASEC values for most SSMs and PCMs (i.e., 1,365-2,251 kJ/kg) are comparable to energy consumption of systems using TCMs (i.e., 1,350-2,060 kJ/kg). This comparison excludes TCMs such as magnesium sulfate, magnesium chloride, and calcium sulfate which perform at lower ASEC values (i.e., 954-973 kJ/kg) and lithium bromide which performs at higher ASEC value (i.e., 4,483 kJ/kg) because of their high and low discharge temperatures, respectively. Yet, the three TCMs with high discharge temperatures (magnesium sulfate, magnesium chloride, and calcium sulfate) decrease ASEC by nearly 30%: a significant energy savings that make high discharge temperature TCMs more promising for waste heat storage.

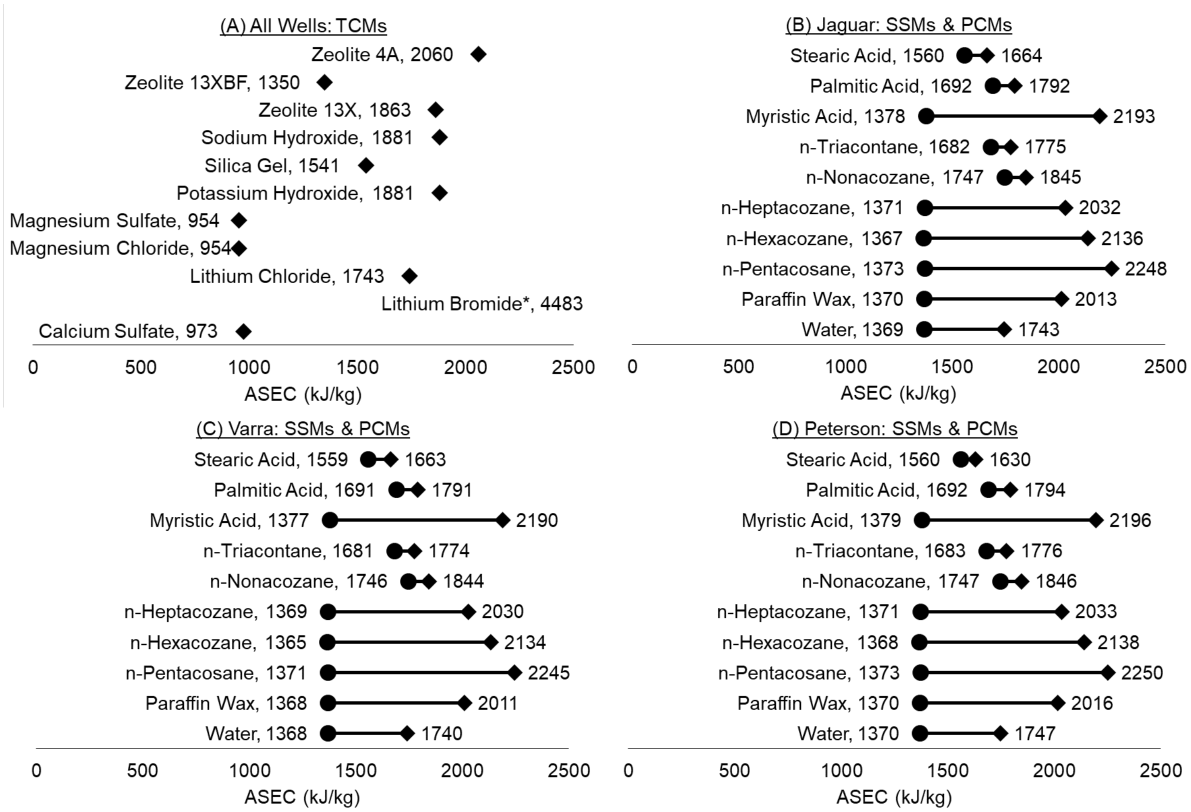

Figure 7: Apparent specific energy consumption for storage materials at different wells. A) For thermo-chemical storage materials, performance is constant at all wells. Lithium Bromide, marked with an asterisk, has a discharge temperature lower than 60°C and is not a viable option for waste heat storage when higher critical operating temperatures are used. Lithium Bromide also has an apparent specific energy consumption value of 4483 kJ/kg, which is beyond the scale of these plots. Sensible storage materials and phase change materials perform differently depending on wells and critical operating temperature. The average (B, Jaguar well), conservative (C, Varra well), and optimistic (D, Peterson well) scenarios are shown. The sensitivity of performance from change in critical operating temperature (40 to 60°C) is represented with the bars. Lower apparent specific energy consumption (circles) is associated with a higher critical operating temperature. Higher apparent specific energy consumption is indicated by a diamond at the lower critical operating temperature. As the discharge temperature of TCMs does not change as heat is removed, the ASEC is only dependent on the material type but not the well or the operational condition of membrane distillation and therefore only have one apparent specific energy consumption value.

By comparing the ASEC values from Figure 7 to the calculated critical (i.e., maximum) SEC at a well, it can be determined directly if the proposed treatment system will be capable of achieving complete treatment of FPW. The minimum GOR can be converted to critical SEC at any well by dividing the latent heat of vaporization for water by the minimum GOR (Figure S2). If the ASEC is above the critical SEC, full treatment is not possible. For example, the critical SEC of the Jaguar well is 1,111 kJ/kg. By looking at the ASEC values from the Jaguar well (Figure 7), it can be concluded that only TCMs such as magnesium sulfate, magnesium chloride, and calcium sulfate are capable of meeting the FPW treatment demands. This conclusion is confirmed in Figure 5, as only the TCMs with very high discharge temperature are capable of achieving full FPW treatment. The critical SEC of the Peterson well is 2,965 kJ/kg, and thus the only TCM that cannot reach full treatment for this well is lithium bromide, which has an ASEC of 4,483 kJ/kg.

The average critical SEC obtained from Figure S2 is 987 kJ/kg, which, in the average case, means only systems using TCMs like magnesium sulfate, magnesium chloride, and calcium sulfate (i.e., the only storage materials with ASEC values under 987 kJ/kg) would be able to meet the FPW treatment demand. For wells with below average minimum GOR values (i.e., 50% of wells), none of the treatment systems could be expected to meet FPW treatment demands by using waste heat from hydraulic fracturing. Among all the materials, only magnesium sulfate, magnesium chloride, and calcium sulfate are able to operate with ASEC values below 1000 kJ/kg. High FPW treatment and lower energy consumption are precursors to a low ASEC value, and therefore these three TCMs enable the highest performance of MD and are the best options available for waste heat storage for use in on-site FPW treatment.

3.3.3. Storage Volumes and Potential for Transportation of Waste Heat from Natural Gas Compressor Stations

Due to the temporal disparity between on-site waste heat generation and FPW treatment demand, we consider another option of waste heat utilization for on-site FPW treatment: the transport of waste heat from natural gas compressor stations, which are more consistent waste heat sources, to the well sites. Therefore, waste heat storage materials need to be transported from the natural gas compressor stations to the well. This strategy needs to be compared to the transport of raw FPW to natural gas compressor stations for off-site treatment [41, 44, 102]. In this case, the number of trucks for the transport of storage material used for waste heat storage must be smaller than the trucks needed to transport raw FPW being treated, because the transportation cost is proportional to the number of trucks transported.

By estimating the inverse volumetric treatment capacity of storage materials for each well (Eq. 18), the viability of transporting waste heat from natural gas compressor stations for decentralized FPW treatment is determined, using the Varra, Jaguar, and Peterson wells as examples for the conservative, average, and optimistic scenarios (Figure 8). The analyses on the remaining wells are shown in the Supporting Information (Table S12-Table S31). The majority of waste heat storage materials result in higher volumes when transporting waste heat for on-site FPW treatment, compared to transporting raw FPW to natural gas compressor stations for centralized treatment. However, three TCMs were identified with the potential to significantly reduce the transportation volume: calcium sulfate, magnesium chloride, and magnesium sulfate. In the average case (i.e., at the Jaguar well), for example, these TCMs have volumetric ratios of storage materials to treated FPW between 0.29 and 0.63. When weight is considered, the transportation ratios for these three materials increase to 0.29-0.71. In such scenarios, transporting waste heat, rather than FPW, could save up to 70% of transportation cost with the use of these appropriate TCMs for waste heat storage and transportation for decentralized FPW treatment. These results also indicate the importance of appropriately selecting thermal energy storage materials when storing waste heat to power on-site FPW treatment.

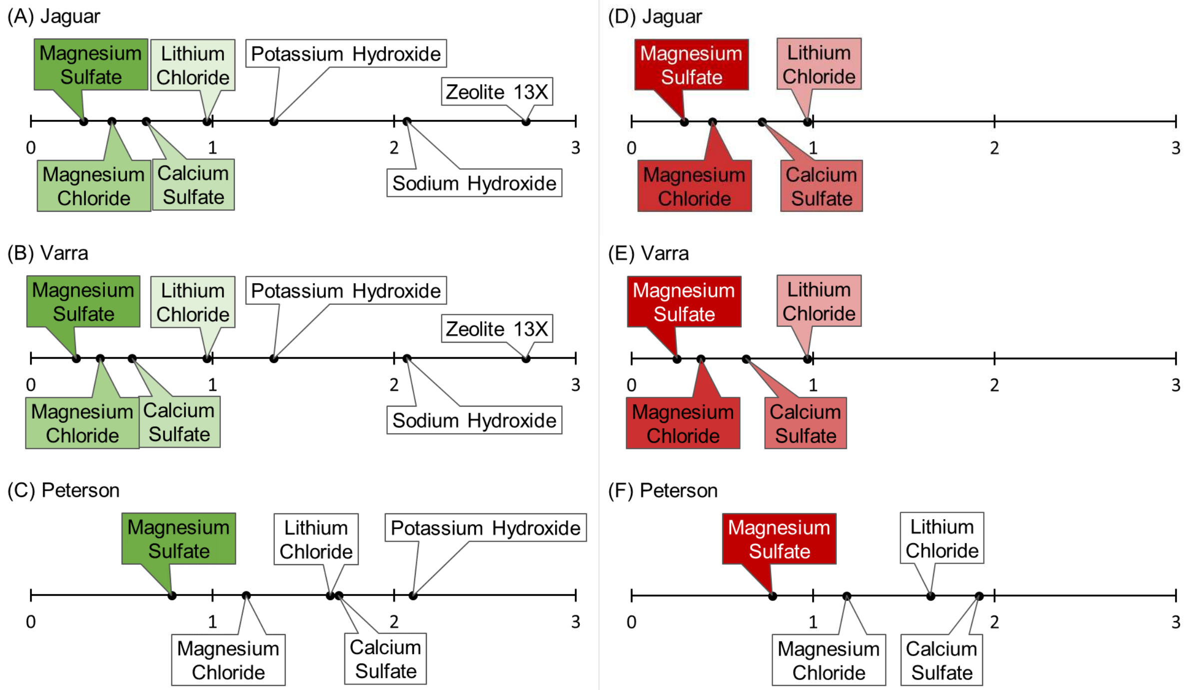

Figure 8: Volumetric ratio (A-C, green) and transportation ratio (D-F, red) of waste heat storage material to raw flowback and produced water treated. For no wells would it be efficient to transport waste heat from natural gas compressor stations using phase-change materials or sensible storage materials when compared to the transport of raw flowback and produced water to natural gas compressor stations for centralized treatment. At the Jaguar (A) and Varra (B) wells, four thermo-chemical materials (magnesium sulfate, magnesium chloride, calcium sulfate, and lithium bromide), highlighted in green (where a darker color of green denotes a material with better volumetric treatment capacity), require lower volumes of storage material than the volume of raw wastewater for transportation. At the Peterson (C) well, only magnesium sulfate is able to reduce the transportation volume. With the added consideration of weight restrictions, the transportation ratio of materials at the Jaguar (D) and Varra (E) wells are not significantly affected, but the Peterson (F) well has no options for waste heat transportation. Materials with a ratio higher than 3 are not represented visually in the figure. Values for other wells are documented in the Supporting Information (Table S12-Table S31).

3.4. Conclusions

This study presents comprehensive analyses of waste heat collection, storage, and utilization for use in FPW treatment by membrane distillation with thermodynamic modeling. Our model was used to evaluate and compare three different scenarios: utilization of waste heat from hydraulic fracturing for on-site FPW treatment, utilization of waste heat from natural gas compressor stations for on-site FPW treatment, and utilization of waste heat from natural gas compressor stations for off-site FPW treatment. The first two scenarios require the storage of waste heat to overcome temporal and spatial disparities in waste heat availability and FPW treatment demand. The second scenario also requires the transportation of stored waste heat from natural gas compressor stations to the site of FPW production. The third scenario is used to compare the potential cost of FPW transportation to natural gas compressor stations with that of the second scenario. These three scenarios were considered for the treatment of FPW using membrane distillation for 20 wells in the Denver-Julesburg Basin and 21 waste heat storage materials.

Results showed that waste heat storage material selection is an important factor when leveraging waste heat for FPW treatment by membrane distillation, with the type of storage materials determining the utilization of waste heat and treatment capacity by membrane distillation. By tracking the change in temperature and energy content of the storage material throughout FPW treatment, we discovered that SSMs are disadvantageous compared to PCMs for waste heat storage due to the addition of latent heat storage in PCMs. Moreover, TCMs, which operate at constant temperatures, are capable of outperforming both SSMs and PCMs when TCMs with high (90°C) discharge temperatures are used. Furthermore, the use of SSMs and PCMs limits the maximum waste heat utilization, a consequence of the critical temperature gap, which renders at least 11% and up to 83% of collected waste heat unusable by the membrane distillation treatment system.

This work, for the first time, quantifies the overall energy consumption of membrane distillation under continually changing conditions by calculating the apparent specific energy consumption. Comparing the minimum GOR (or critical SEC) of the wells to the attainable ASEC values for the proposed treatment systems, the average well could expect to see 100% FPW treatment when using calcium sulfate, magnesium chloride, or magnesium sulfate. These three TCMs enable the highest performance of MD and are the best options available for waste heat storage to be used in on-site FPW treatment. Furthermore, these three TCMs have transportation ratios between 0.29 and 0.97 for the average scenario of waste heat availability and FPW treatment demand, indicating that it is cost effective to transport the waste heat rather than the FPW when leveraging waste heat from natural gas compressor stations. In treatment scenarios which use these three TCMs as waste heat storage material, transporting waste heat rather than FPW could save up to 70% of transportation costs for FPW treatment.

Looking back at Figure 2, we see that both treatment scenarios for decentralized treatment are viable. Our results showed that decentralized treatment using stored waste heat from the hydraulic fracturing process (Figure 2A) is viable in cases where sufficient waste heat generation is present. We also see that waste heat transportation (Figure 2B) is an option for further consideration. When compared to wastewater transportation (Figure 2C), waste heat transportation could decrease transportation costs by up to 70%. In both decentralized treatment scenarios, thermo-chemical storage materials are the best options for waste heat storage. The next steps in evaluating the feasibility of waste heat utilization for FPW treatment is to conduct a thorough economic analysis of the options for waste heat utilization and transportation throughout the Denver-Julesburg Basin, which includes system design and considerations such as system scale, and brine management.

4. TARGETING SUSTAINABLE DESALINATION SOLUTIONS: A TECHNO-ECONOMIC AND LIFE CYCLE APPROACH TO GUIDING ZERO LIQUID DISCHARGE DESALINATION[6]

4.1. Introduction

The management of hypersaline brine is a prominent challenge that constrains the sustainability of multiple industries (e.g., desalination, power, and resource extraction industries) [103-108]. Zero liquid discharge (ZLD) has been gaining increasing interests as an ideal brine management approach [14, 109, 110]. To pursue ZLD, mechanical vapor compression (MVC) coupled with a brine crystallizer has long reigned as the state-of-the-art technology [14, 37, 57, 108, 111-113]. MVC is a well-established evaporative technology that utilizes latent heat recovery to reduce electricity consumption to 30-40 kWh/m^3 [6, 33, 57, 111]. However, MVC's prominence comes at a substantial cost because of its high capital investment required for expensive anti-corrosive materials and its high electricity consumption even after thermal energy reuse [14, 33, 37, 57, 113, 114]. Recognizing the necessity to drive down the costs and energy intensity associated with existing ZLD options, there has been a notable shift in focus towards membrane-based alternatives [5, 31, 41, 43, 47, 57]. One promising contender within this domain is membrane distillation (MD), a thermally driven membrane technology that shows promise in reducing equipment costs due to its lower operational temperature while effectively treating high-salinity wastewater

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[6] Under Review Submission: B. M. Grauberger, G. M. Cole, T. Tong, S. Lin, J. C. Quinn, T. Bandhauer, " Targeting Sustainable Desalination Solutions: A Techno-economic and Life Cycle Approach to Guiding Zero Liquid Discharge Desalination," Journal of Cleaner Production

[5, 31, 44, 47, 84, 103, 106, 115, 116]. However, MD remains energy-intensive due to thermal energy loss through transmembrane heat transfer and its competitiveness against MVC hinges on the availability of waste heat as an energy source [31, 47, 84, 111]. Furthermore, as with MVC, it is required to pair an energy-intensive crystallizer (>50 kWh/m^3, [14]) with MD when targeting ZLD, adding more complexity and costs.

Recently, electrodialytic crystallization (EDC) has emerged as a new technology that enables ZLD through a non-evaporative approach [57]. In EDC, ions in the feedwater are constantly migrating to a recirculated brine stream under an electric field, which increases the brine concentration beyond the salt solubility limit and thus induces salt crystallization. EDC achieves brine crystallization without evaporation, avoiding the energy-consumptive phase transition and thus having the potential to reduce electricity consumption in comparison to thermal technologies such as MVC and MD. EDC has exhibited a capacity to outcompete MVC paired with a crystallizer for energy efficiency, signifying a leap towards a more sustainable and cost-efficient approach of ZLD [57]. EDC also carries the potential to alleviate the financial burden associated with the use of anti-corrosive materials in MVC, because it is able to operate at ambient temperatures [57]. Furthermore, EDC is aligned with the global movement toward decarbonization through sustainable electrification [117-119]. Electrifying ZLD using EDC reinforces its position as a compelling choice for future ZLD development.

As EDC is in its infant stages of development, researchers can benefit from identification of high impact research directions to optimize research efforts and fast-track the development of EDC. As recently suggested by Lee et al. [111], analyzing the economic viability of emerging technologies at the water-energy nexus is essential to the feasibility of the technologies for potential upscaling and commercialization. Chiefly, techno-economic analyses (TEA) and life cycle assessments (LCA) are useful tools that can be used to inform decisions made in early development, which have the potential to significantly impact the economic viability and environmental sustainability of fully developed systems [106, 111, 120]. So far, TEA and LCA have been applied to assessing the economics and environmental impacts of emerging brine treatment technologies such as MD [37, 47, 121-124]. However, these studies have predominantly focused on comparing the economic and environmental competitiveness to those of existing technologies. Historically, using the capabilities of TEA and LCA tools to identify high-impact research directions have only attracted attentions recently [116, 120, 125]. Furthermore, to the best of our knowledge, parallel comparisons of multiple ZLD technologies by TEA and LCA with sensitivity and scenario analysis have not been performed so far.

In this work, we performed TEA and LCA both to compare EDC with existing ZLD technologies and to determine critical areas that have the highest impact for improving the feasibility of EDC in future research. This article begins by outlining technical models for EDC, MVC paired with a crystallizer (referred to as MVC+C), and MD paired with a crystallizer (referred to as MD+C). The MVC+C system serves as the state-of-the-art, or baseline, ZLD technology that is already established in industry. EDC must be competitive with the MVC+C system to progress to higher levels of development. Simultaneously, EDC is competing with the MD+C system as an alternative membrane-based ZLD technology. Additionally, the MD+C system is considered with both electrical resistive heating and waste heat as energy sources. The ZLD system evaluated with waste heat use is annotated as “MD+C w/ WH”. The models for these four ZLD technology systems will then be coupled with cost and life cycle impact models to evaluate and compare their economic and environmental competitiveness through TEA and LCA methodologies. Afterwards, a sensitivity assessment is conducted to identify factors that highly affect the economic and environmental impacts of each technology. The findings of this work demonstrate the value of TEA and LCA methodologies in the identification of research directions that should be prioritized in developing EDC as a competitive ZLD technology.

4.2. Methods

The technologies were compared on an economic and environmental basis. First, technical models were developed to provide mass and energy flows (i.e. life cycle inventory data). After defining the functional unit as a basis for comparison, the cost and environmental impact models were integrated to assess the economic viability and environmental sustainability based on a set of performance indicators. In the final step, a sensitivity assessment was completed to add context to the results. Specifically, sensitivity assessments were used to identify which operating conditions have the highest effect on the economic and environmental competitiveness of each technology and allowed for prioritization of future research objectives. The specific methodologies for each of these five steps are outlined in the follow sub-sections.

4.2.1. Technical Performance Models

Creating performance models was the first step in conducting either TEA or LCA. These models provided mass and energy flows (i.e., life cycle inventory data) of the systems. These models also allowed us to conduct local sensitivity assessments on given model inputs (i.e., operational parameters or conditions). To compare the four ZLD systems, 4 separate thermodynamic models were integrated to determine technical performance. The major inputs to modelling are listed in Table 5. These models are discussed briefly here, but further detail is provided on these models in Section Appendix:S.4.1 of the Supporting Information (SI).

First, the MVC model was created in the process simulation software, Aspen Plus. The process flow diagram for MVC is show in Figure 9. MVC is a thermal desalination technology which works by evaporating water from brine streams. Electrical energy is provided to a compressor, which recovers the steam produced in the evaporator by increasing its temperature and pressure so it can be reused to evaporate the water from the incoming brine in the evaporator. The heat from the compressed vapor, which is compressed to a saturation temperature and pressure above that of the operating vapor temperature and pressure, defined by the evaporator temperature difference (Table 5), is transferred through the evaporator into the brine, causing evaporation of water. The evaporator temperature difference is an important variable to consider, as it determines both the compressor power and the evaporator size necessary for operation [34, 126]. However, the compressor energy consumption and the evaporator size are optimized in opposite relations to the evaporator temperature difference, resulting in an optimal temperature for minimizing the combined cost of the evaporator and lifetime energy costs [34, 126]. The operating vapor temperature of the MVC system is set in a way that puts the evaporator under vacuum, allowing for lower operating temperatures throughout the system. Pre-treatment chemicals (discussed further in the SI) are added to the MVC feedstock before entering the evaporator. All clean water produced by MVC is dosed with chlorine as a final disinfectant.

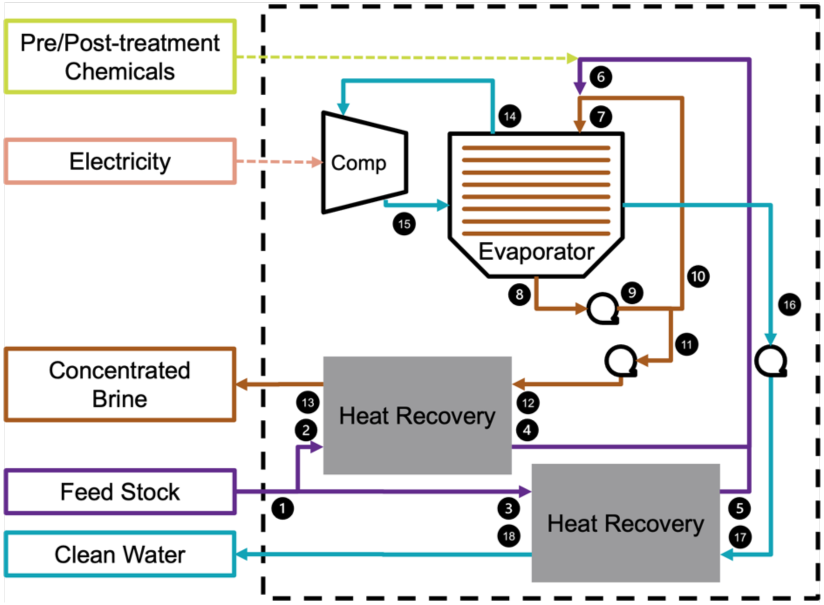

Figure 9: Process Flow Diagram of Mechanical Vapor Compression. Feedwater (stream 1) is preheated in two in-line heat recovery units. The preheated feedwater (stream 6) is fed into an evaporator, where compressed water vapor (stream 15) induces water in the feedwater to evaporate, and a clean water vapor (stream 14) and concentrated brine (stream 18) are produced. Stream 14 is compressed toa a higher pressure to provide heat to the evaporator. Additional heat from the condensed vapor (stream 16) is recovered to preheat stream 3 and clean water is produced (stream 18). A portion of the concentrated brine (stream 12) also provides preheating to stream 2 before leaving the system as a concentrated brine product (stream 13).

The crystallizer (Figure 10), which was paired with the MVC and MD technologies in their respective ZLD systems, was modeled with Aspen Plus software. MVC and MD both provided a nearly saturated brine to the crystallizer. The crystallizer operates similarly to the MVC unit but includes a centrifuge which allows for solids separation. Additionally, heat is not directly added to the brine in the evaporator to avoid crystal buildup within the crystallizer. Rather, the brine temperature is increased in a heater, before entering the evaporator. The evaporator is in vacuum, which flash-evaporates water vapor from the brine upon entering. A portion of the further concentrated brine, which contains a portion of crystallized salts, is diverted to the centrifuge to separate the crystallized salts. Liquid brine from the centrifuge is recirculated to the brine inlet. Recirculation of brine in the crystallizer allows for additional thermal efficiencies in the system. The recirculation rate (Table 5) of the crystallizer defines that the volumetric flow of streams 13 and 15, combined, will be *r* times higher than that of stream 1 (Figure 10), where *r* is the recirculation rate. The clean water produced from the crystallizer is dosed with chlorine to disinfect the water before use in other applications.

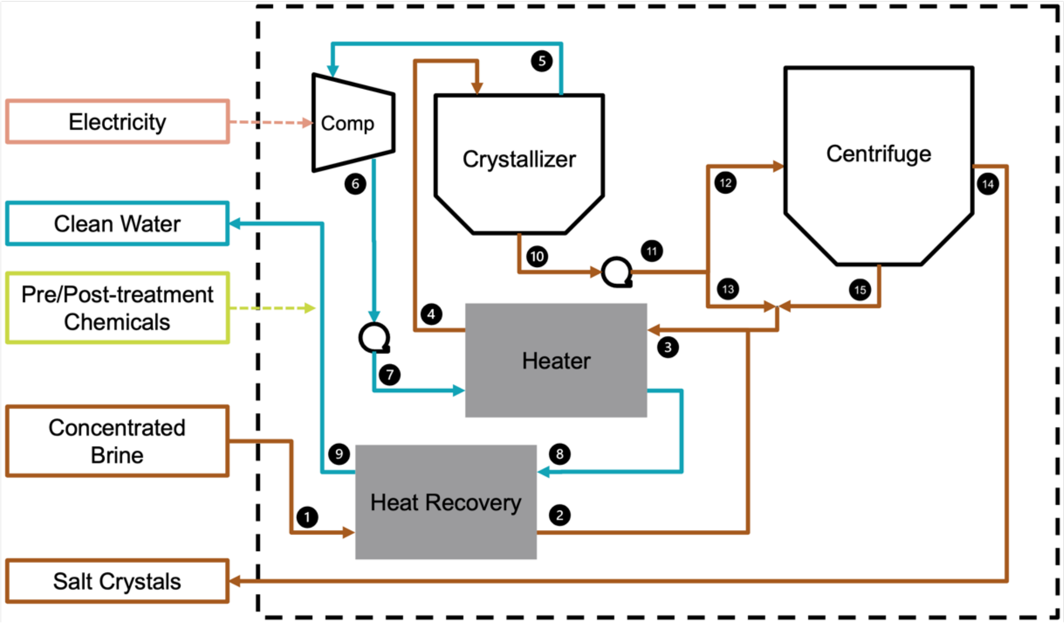

Figure 10: Process Flow Diagram of a Crystallizer. Concentrated brine (stream 1) is preheated in a heat recovery unit, then heated using compressed vapor (stream 7) in the heater. When the heated brine (stream 4) enters the evaporator, pressure differences induce evaporation and a clean water vapor (stream 5) and a brine with crystalized salts (stream 10) are produced. A portion of stream 10 is fed into a centrifuge, which removes the crystallized salts (stream 14) from the saturated brine (stream 15). The clean water vapor (stream 5) is compressed in the compressor to provide a high temperature stream for heating (stream 6).

Existing models were used to determine the performance of MD and EDC. The process flow diagrams for these technologies are provided in in Figure 11 and Figure 12, respectively These models have been published by Robbins et al. and Zhang et al., respectively [5, 57]. Similarly to the models created in Aspen Plus for this work, major inputs used in these existing models are listed here, in Table 5. As with all other technologies, all clean water produced in EDC and MD are treated with chlorine as a disinfectant.

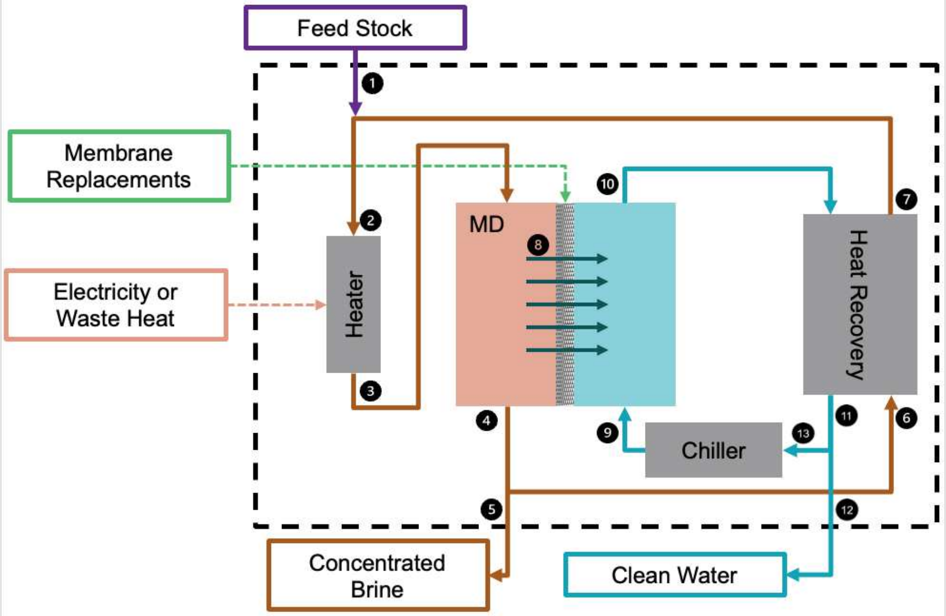

Figure 11: Process Flow Diagram of Membrane Distillation. A feedwater (stream 1) is heated using an electric resistance heater and enters the hot side of the membrane distillation module. Water vapor transfer through the hydrophobic membrane (stream 8) is induced though the temperature difference, and resulting pressure difference, across the membrane. A portion of heat lost through heat transfer in the membrane is recuperated in the heat recovery unit. Membrane distillation produces a clean water (stream 12) and a concentrated brine (stream 5).

MD is a thermally driven membrane technology that operates by creating a temperature difference across a hydrophobic membrane. The temperature difference drives a vapor pressure difference across the membrane, and water from the heated side of the membrane will evaporate at the surface of the membrane and travel through to condense in the clean, cool-water flow. The temperature to which the water is heated (i.e., the inlet temperature (Table 5), or the temperature of stream 3) has a large effect on the performance of MD [5, 84]. Higher temperatures result in higher water vapor flux across the membrane, and decrease the specific energy consumption (SEC), and necessary membrane area for the system. To maintain temperature differentials across the membrane, electricity or waste heat is provided to the heater and cold water flows are cooled in the chiller to atmospheric temperatures. When modelling the use of waste heat, there is additional consideration of the waste heat collection and delivery technology. In modelling, the recovery rate of the MD system is defined. This value represents the percentage of feedwater volume that is removed by the MD technology. Lower recovery rates are easier to achieve for the MD technology. However, in the ZLD system (i.e., when paired with a crystallizer) more of the desalination load is shifted to the crystallizer.

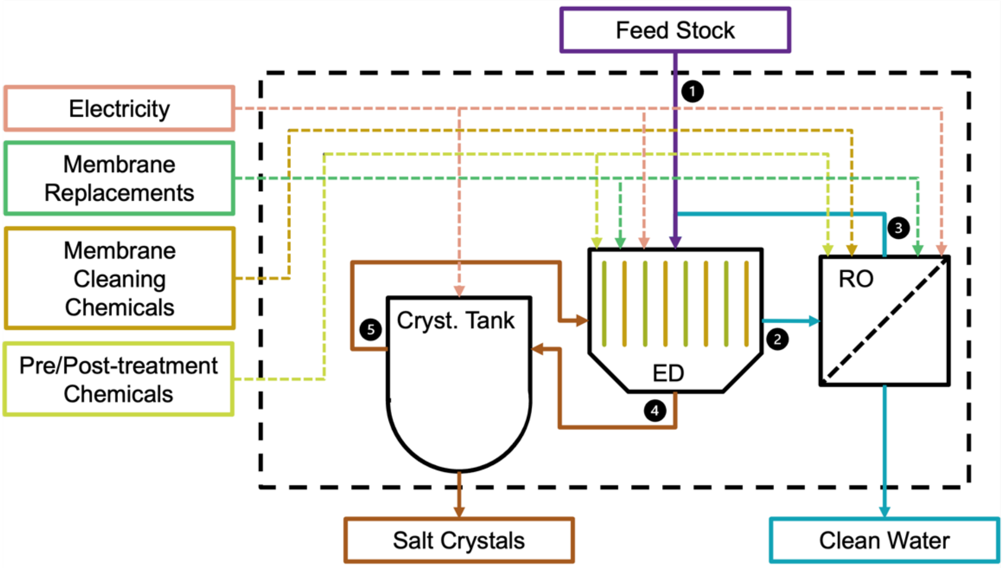

Figure 12: Process Flow Diagram of an Electrodialytic Crystallizer. Feedwater (stream 1) is fed into the electrodialysis unit and is split into a saturated brine (stream 4) and a diluted brine (stream 2). Stream 2 is fed into a reverse osmosis unit which produces clean water, and a brine (stream 3), which is re-fed into the electrodialysis unit. Stream 4 is fed to a crystallization tank, where salt crystals are settled out and collected. The outlet of the crystallization tank (stream 5) is refed to the concentrated flow within the electrodialysis unit.

EDC, the technology of focus for this work, is unique in that it does not use thermal desalination. Rather, EDC pairs electrodialysis (ED) and reverse osmosis (RO) together to create salt crystals and clean water, respectively [57]. ED is a membrane technology which drives salt ion transfer through membranes by providing an electrical potential to the system. By strategically placing ion exchange membranes (IEMs), channels of concentrated and diluted brines are produced by the ED system. The concentrated brines (Stream 4, Figure 12) are sent to a crystallization tank, where temperature of the stream is decreased to induce salt crystallization by lowering solubility. The diluted brine produced in ED is sent to a RO unit, which uses osmotic pressure to induce water transfer through a membrane, producing clean water. The re-concentrated brine from the RO unit is then fed back into the ED unit for further concentration. The performance of the ED system is defined by feed stock flowrate and salinity, current density, and crystal yield (Table 5). Current density of the ED module determines the potential of ion transfer. Subsequently, it largely affects the necessary IEM area and electricity consumption of the system. Values used for current density in this work are based on the experimental results from batch operation in Zhang *et al.* [57]. Crystal yield is defined as the ratio of actual brine total suspended solids (i.e., crystal formation) and the theoretical maximum total suspended solids for the brine. Crystal yield in this work is set to the range of testing results to allow a conservative estimate of EDC operation at scale and under continuous operation rather than lab-scale batch operation. The crystal yield of the ED system is based on experimental results from Zhang *et al.* [57]. Further modelling details are shared in Section Appendix:S.4.1 of the SI.

Table 5: Inputs for Mechanical Vapor Compression, Electrodialytic Crystallization, Membrane Distillation, and Crystallizer Models

Model	Variable	Value	Units	Notes/References
All	Inlet Flowrate	900	m^3/day	The baseline value represents a full-scale desalination plant. Desalination facilities can range from volumes of 15-90,000 m^3 per day [127, 128]. This number attempts to capture the volume of effluent from a mid-sized desalination facility.
	Inlet Salinity	68,500	ppm	Brines from brackish and seawater desalination plants have a salinity which reached 70,000ppm, or the limiting salinity of RO [14].
	Lifetime	15	$years$	[129]
	Cost of Energy	0.073	$\$/kWh$	[130]
MVC	Compressor Efficiency	0.7	-	[131, 132]
	Operating Vapor Temperature	60	$^{\circ}C$	This value represents the temperature in the evaporator.
	Evaporator Temperature Difference	10	$^{\circ}C$	This value represents the temperature difference between the low-pressure vapor being produced in the evaporator, and the high-pressure vapor leaving the compressor, which is providing the heat in the evaporator. The values from literature range from 2°C to 10°C, though lower values are shown to result in lower electricity consumption, but raise capital expense due to increases in evaporator size [34, 126]. Therefore, we chose to use 10°C, which has shown to provide lower combined cost of the evaporator and electricity costs [34, 126].
EDC	Current Density	200	amp/m^2	The experiments run in Zhang *et al.* ranged current density from 200 to 600 amp/m^2. The lower current densities resulted in lower crystallization rates in ED, so the average current density value used in this work, in an attempt to provide conservative predictions in performance, was set to 200 amp/m^2 [57].
	Crystal Yield	0.6	-	The experiments run in Zhang *et al.* are in batch-mode. This model is based on continuous operation and is expected to have more efficient performance [57].
	RO Membrane Replacement Factor	25	$\%/year$	The replacement factor represents the amount of membrane being replaced every year. Another way to represent the membrane replacement factor would be as a membrane lifetime. In this case, a membrane replacement factor of 25% per year equates to a membrane lifetime of 4 years [133].
	Ion Exchange Membrane Replacement Factor	8	$\%/year$	As above, an 8% per year membrane replacement factor equates to a 12.5 year membrane lifetime [133].
	Cost of Ion Exchange Membrane	100	$\$/m^2$	[133-137]
	Crystallization Tank Retention	12	$hours$	Longer retention time will allow for more crystallization. However, these crystallization kinetics are not accounted for in this model. This value is used for sizing and costing the tank, in this work.
	Temperature Drop in Crystallization Tank	2	$^{\circ}C$	A higher temperature drop from the inlet temperature of the crystallization tank to the bulk temperature of the crystallization tank will allow for more crystallization, as the solubility limit of a solution is higher at higher temperatures. Decreasing the temperature of brine in the crystallization tank will induce crystallization by lowering the solubility limit.
MD	Inlet Temperature	65	$^{\circ}C$	[5]
	Recovery Rate	62.5	%	[5]
Crystallizer	Compressor Efficiency	0.7	-	[131, 132]
	Operating Vapor Temperature	60	$^{\circ}C$	This value is the pressure of the vapor under vacuum before the compressor [138].
	Heater Temperature Difference	1	$^{\circ}C$	This value represents the temperature difference between the saturation temperature of the condensed liquid leaving the heater and the low-pressure liquid having been heated in the heater, which is providing the heat for evaporation in the in the crystallizer. [138]
	Crystallizer Recirculation Rate	100	-	The crystallizer recirculation rate determines the rate of flow through the crystallizer. This value of 100 means that circulation through the crystallizer is 100 times that of the inlet flow to the system. Additional flow is used to maintain thermal efficiencies in the system. [138]

4.2.2. The Functional Unit

In this work, we evaluated technologies that desalinate brines. The purpose, or function, of these systems is to desalinate a volume of brine. As such, all impacts and/or costs were attributed based on volume of clean water produced. By normalizing impacts and/or costs against this functional unit (i.e., per cubic meters of clean water produced), we were able to compare systems across all operational parameters. In this work, TEA results were reported in cost per cubic meter of clean water produced. This normalization of cost was called the "levelized cost of water" (LCOW). LCA results were also normalized to cubic meters of clean water produced. For example, global warming potential (GWP) was reported in units of $kg\ CO_{2,eq}/m^3$, etc.

4.2.3. Calculating Costs – Techno-economic Analysis

A TEA was completed by evaluating system costs. Yearly expenses were calculated, loan paybacks were considered, and all values were normalized through a discount rate, which encompasses the time-value of money. By following these methods, the total lifetime costs can be compared on similar basis. In this case, the basis is in the value of the 2022 United States Dollar.

4.2.3.1. Scope

For this work, both capital and operational expenses were included in the calculation of LCOW. No end-of-life or disposal costs were included. As described above in Section 4.2.2, the functional unit of our analysis is a cubic meter of clean water produced, and all results were levelized against this functional unit.

4.2.3.2. Expense Models

Section Appendix:S.4.2 of the SI shares cost models for equipment and variable costs of the four technologies. Costs were calculated in reference to the value of the 2022 United States Dollar. All technologies' capital expenses were split into primary equipment, secondary equipment, other direct, and indirect costs. Primary equipment costs were those associated with the primary technology of the system—those which are the defining technology of the system. Secondary equipment costs were those associated with the secondary technology in each system, or those which support the primary technology in achieving ZLD. For the MVC+C, EDC, and MD+C systems, primary technologies are MVC, ED, and MD, respectively. As such, the secondary technologies are the crystallizer, RO, and crystallizer, respectively. Table S41 in the SI shares further breakdowns of each cost for the four ZLD technologies.

For all technologies, other direct costs (i.e., warehouse costs, site development, and additional piping) were calculated as 17.5% of total equipment costs. Indirect costs (i.e., prorateable expenses, field expenses, home office and construction fees, project contingency, and other costs) were calculated as 60% of combined equipment and direct costs.

Operational expenses were split into variable and fixed operating expenses. Variable costs included electricity costs (split into primary and secondary), and all other variable costs such as membrane replacement and chemical consumption (again, split into primary and secondary categories). Fixed operating costs included insurance and maintenance. Insurance was calculated as 0.7% of total initial capital investment per year, and maintenance as 3% of total equipment costs per year.

Table S41 in the SI shares the calculated equipment and variable costs for every technology in its average operating scenario.

4.2.3.3. Discounted Cashflow Rate of Return

TEA uses the previously calculated capital and operational costs and evaluates them through a discounted cashflow rate of return (DCFROR) analysis. The DCFROR analysis was used to determine the LCOW for each system. This analysis enabled costs throughout the lifetime of a technology to be mapped yearly, allowing for the initial capital investments, as well as operational expenses to be appropriately allocated to the functional unit over the lifetime of the technology using an internal rate of return. Revenue, taxes, loan interest, loan payments, buildout periods, start-up operations, and depreciation were considered in the DCFROR. The discount rate considered in the analysis was 10%, which matches industrialized projects [139]. Inputs used for the DCFROR analysis are shared Table S42 in the SI.

4.2.4. Determining Environmental Impacts – Life Cycle Assessment

4.2.4.1. Goal and Scope

To compare systems in a consistent manner, we have followed the standardized methodology for LCAs [140].The first step of the LCA, as laid out in the International Standards Organization (ISO) standards 14040, was to define the goal and scope of the assessment [140]. Following these standards, we defined our system boundary to include only the operation stage of the desalination technologies. Though we could have included the emissions associated with initial equipment purchases for the systems in our analysis, we decided to focus on operations, as most impacts of industrial systems could be attributed to the operational phase [74]. No end-of-life impacts were included. As described above in

Section 4.2.2, the functional unit of our analysis was a cubic meter of clean water produced, and all results were levelized against this functional unit.

4.2.4.2. Life Cycle Inventory Analysis and Impact Assessment

The technical models establish a life cycle inventory for the systems. Databases were used to assess the life cycle impacts of upstream and downstream processes included in the life cycle inventory. The LCA completed in this study used data supplied by the EcoInvent v3.8 database, using cutoff analysis [141]. The information was accessed through the openLCA software 1.11 [142]. Additional information on the use of these resources can be found in Section Appendix:S.4.3 of the SI.

We are reporting all impacts included in the Tool for Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI): acidification, eutrophication, carcinogenics, non-carcinogenics, ecotoxicity, smog, respiratory effects, fossil fuel depletion, ozone depletion, and GWP [143]. OpenLCA was used to determine the TRACI impacts from each inventory item from the life cycle inventory. Life cycle impact assessment was completed using a spreadsheet model which allocated impacts of technologies based on their use of each inventory item and its respective impacts. All final reported impacts are normalized against the functional unit. Additional information on the impacts of emissions sources can be found in Section Appendix:S.4.3 of the SI.

4.2.5. Scenario and Sensitivity Assessments

Two types of assessments were completed in this work to determine high-impact operating parameters: a scenario analysis, and a local sensitivity assessment. These two methodologies served to inform us on different aspects of potential system impacts.

The scenario analysis identified the potential impacts of a technology in a situation where the system was allowed to perform under its best capabilities, or where it may be strained under operating conditions. In the scenario analysis, all variable inputs were set to a value which benefits (i.e., optimistic scenario), conflicts (i.e., conservative scenario), or represents the average performance of the technology [144] (Table 6). Operational scenario values were primarily selected based upon the average, or expected, operational condition of the technologies. That is, the average operational scenario was set using available data from full-scale applications (in the case of MVC and the crystallizer), and from expected full-scale performance (in the case of EDC and MD). When available, further data was used to represent values of conservative and optimistic operational conditions. In some cases, only values for optimistic or conservative scenarios were distilled from literature, in which case the identical range from the average scenario value was used to fill in the missing data. In the case of universal input variables (i.e., treatment rate, brine salinity, and cost of energy), the conservative and optimistic scenario values were varied by 20% of the average scenario value.

By evaluating each of these three scenarios, we identified the range of impacts that could be expected from these emerging technologies. Further, by comparing these technologies, the potential for new systems (i.e., EDC or MD+C) to compete with existing technologies (i.e., MVC+C) was quantified. It is worth noting that pre-existing, well researched, and well-tested technologies will be less sensitive to scenario analysis because the range of operating parameters is better understood and defined [145, 146]. The variables which contribute to the largest ranges in results are those which should be focused on in future development to reduce uncertainty.

Local sensitivity assessments (a.k.a., one-at-a-time sensitivity assessments) were used in this work to identify operating conditions (i.e., input variables) which contribute the highest to changes in overall impacts [147, 148]. For each of the scenarios, the inputs listed in Table 6 were adjusted ±10%, one at a time. The resulting change in LCOW and environmental impacts was recorded. The variables were then ranked by their effect on the final impact values (i.e., those that result in the highest change to end-results). The variables with the highest potential to change the impacts of technologies are those which should be focused on in future development, as they have the highest potential to reduce costs and environmental impacts through optimization.

Table 6: Scenario Inputs Mechanical Vapor Compression, Electrodialytic Crystallization, Membrane Distillation, and Crystallizer Models

Model	Variable	Average Value	Conservative Value	Optimistic Value	Units	References
All	Inlet Flowrate	900	720	1080	m^3/day	[127, 128]
	Inlet Salinity	68,500	82,200	54,800	ppm	[14]
	Lifetime	15	10	20	$years$	[129]
	Cost of Energy	0.073	0.0876	0.0584	$\$/kWh$	[130]
MVC	Compressor Efficiencies	0.7	0.6	0.8	-	[131, 132]
EDC	Current Density	200	100	300	amp/m^2	[57]
	Crystal Yield	0.6	0.4	0.8	-	[57]
	RO Membrane Replacement Factor	25	33	20	$\%/year$	[133]
	Ion Exchange Membrane Replacement Factor	8	10	5	$\%/year$	[133]
	Cost of Ion Exchange Membrane	100	150	50	$\$/m^2$	[133-137]
	Crystallization Tank Retention	12	18	6	$hours$	
	Temperature Drop in Crystallization Tank	2	4	0	$°C$	
MD	Inlet Temperature	65	50	80	$°C$	[5]
	Recovery Rate	62.5	75	50	%	[5]
Cryst.	Compressor Efficiency	0.7	0.6	0.8	-	[131, 132]
	Crystallizer Recirculation Rate	100	70	130	-	[138]

4.3. Results & Discussion

The effects of system operating parameters on the LCOW and environmental impacts of different ZLD technologies are analyzed in detail through TEA and LCA. First, the LCOW and environmental impacts of water treatment are calculated for various (i.e., average, optimistic, and conservative) operating scenarios. Further, a local sensitivity assessment is performed for each scenario, where the effects of changes to each operating parameter on cost and environmental impact are measured.

4.3.1. TEA demonstrates that EDC can lower ZLD costs compared to thermal technologies

In the current study, TEA is used to calculate the levelized lifetime costs of four ZLD systems (i.e., MVC+C, EDC, MD+C, and MD+C w/ WH) through a DCFROR. The costs are levelized against the functional unit for reporting (i.e., the treatment of one cubic meter of brine). Results for the LCOW of 24 scenarios are reported in this section. Twelve scenarios share results for crystallization of brines consisting of Na_2SO_4 and the other twelve for NaCl brines, (Figure 13 and Figure S5 in the SI). MVC+C, EDC, MD+C, and MD+C w/ WH are evaluated in the average, optimistic, and conservative operating scenarios.

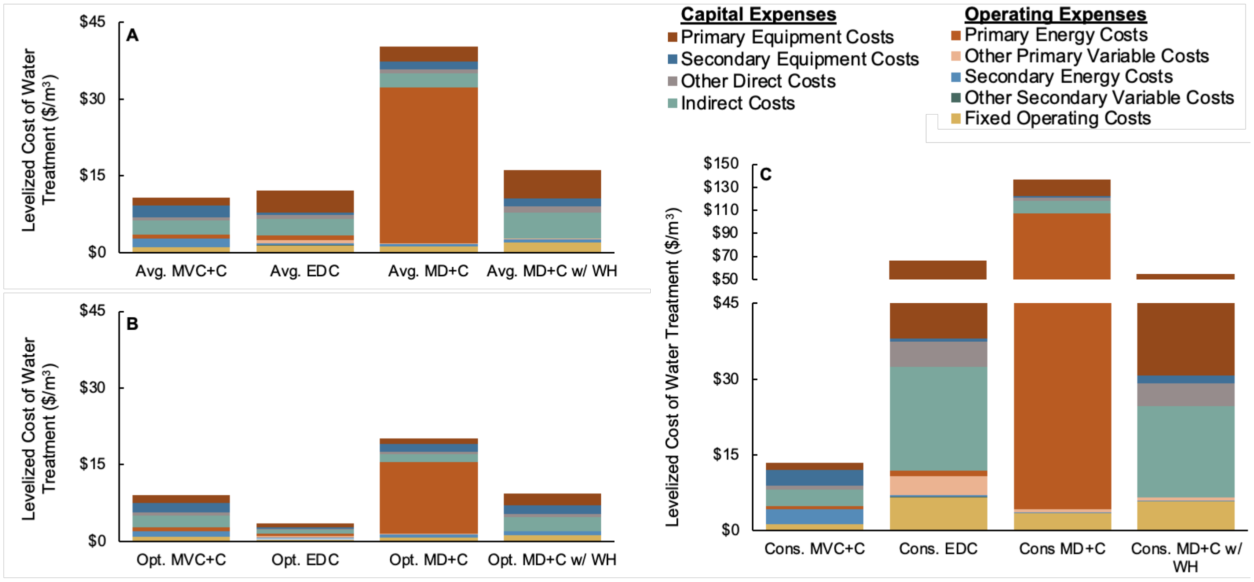

Figure 13: Levelized Cost of Water Treatment for Na_2SO_4 Crystallization. Results are split into the A) average (Avg.), B) optimistic (Opt.), and C) conservative (Cons.) operation scenarios. The cost of electrodialytic crystallization (EDC) changes significantly between the operating scenarios, which displays the unpredictability of EDC performance, and the risk in developing full-scale EDC systems for zero liquid discharge desalination applications. Mechanical vapor compression paired with a crystallizer (MVC+C), membrane distillation paired with a crystallizer (MD+C), and MD+C when using waste heat (MD+C w/ WH) are the other technologies compared.

As shown in Figure 13 (also tabulated in Table S45), EDC, as an emerging ZLD desalination technology, is competitive with the existing baseline technology (i.e., MVC+C) under the average scenario and can outperform MVC+C under the optimistic operating condition. In the average scenario, the operational costs of EDC ($\$3.31/m^3$) and MVC+C ($\$3.52/m^3$) are roughly the same, and the increased LCOW of EDC over that of MVC+C is due to capital investments — the capital cost of EDC is $\$1.52/m^3$ higher than that of MVC+C. This comparison exemplifies the importance of considering capital costs of new technologies. Energy costs of EDC ($\$1.01/m^3$) are less than half of MVC+C ($\$2.38/m^3$), but the equipment costs of EDC are much higher than MVC+C and nullify the cost savings from improved energy efficiencies. Our results demonstrate that energy efficiencies are not the determining factor of LCOW of these ZLD technologies. Rather, an in-depth understanding of the parameters affecting both capital and operating expenses is essential to evaluating the economic feasibility of emerging technologies.

Overall, EDC LCOW in the avenge scenario, though slightly higher than that of MVC+C, shows the potential competitiveness of the EDC for ZLD applications. Furthermore, in the optimistic operating scenario, the LCOW of EDC is lower than that of the baseline technology, MVC+C. This comparison shows EDC has the potential to reduce total LCOW of existing ZLD technologies, not only costs of electricity. Compared to the average scenario, LCOW reductions are seen for both technologies in the optimistic scenario. The majority of LCOW reductions for the MVC+C system are through operational costs, whereas EDC experiences the greatest reductions through capital cost. Specifically, a 23% reduction in operational expenses and 12% reduction in capital costs are seen for MVC+C. The reductions in EDC cost are much larger: a 54% reduction in operational expenses and a 77% reduction in capital costs. Overall, there is less change to the LCOW of MVC+C because there is more understanding about the boundaries of operation in the baseline technology, due to the technical maturity of MVC+C. On the contrary, EDC, as a newly developed technology, has a wider range of operating parameters represented because these boundaries have not been explored individually at scale to improve our understanding of the technology. Though these limits are not yet fully understood, our results exemplify the potential of EDC to outperform MVC+C technologies economically.

However, in unfavorable conditions (i.e., in the conservative operating scenario) EDC has much higher LCOW than that of MVC+C due to the significant increase of primary equipment cost. Such an increase is the result of increases in IEM area necessary for operation. This membrane area increase is due to the decreased current density, and lower crystal yield, which both necessitate higher membrane areas to overcome losses in performance. Furthermore, there is an increase of IEM cost from $\$100/m^2$ to $\$150/m^2$. Because both the membrane areas and membrane costs are increasing, further equipment costs are accrued. Since other cost categories (e.g., other direct cost, indirect costs, and fixed operating costs) are calculated as a percentage of total equipment costs, an increase is also seen in these categories. Once all costs are levelized in the conservative scenario, roughly 63% of the LCOW is directly and proportionally correlated to the cost of IEMs. Similarly, the decrease in EDC LCOW in the optimistic scenario can be largely attributed to lower necessary IEM area and lower IEM costs. Therefore, it is important to reduce the cost of IEMs to enhance the competitiveness of EDC. Because EDC and the use of IEMs in high-concentration treatment scenarios is a relatively new application, research developments could improve both performance and cost of IEMs.

Broadly, we know that it is possible to reduce costs of EDC to be competitive with MVC+C, the baseline technology, if the costs associated with the IEM membrane are reduced. In fact, the optimistic scenario EDC LCOW ($\$3.55/m^3$) is below the costs of MVC+C ($\$9.12/m^3$) by $\$5.57/m^3$. However, there is risk for high EDC LCOW, as shown in the conservative EDC scenario. As research is continued on EDC, and our understanding of the technology improves, the wide range of results between the conservative and optimistic scenarios will converge to be more predictable. From scenario analysis of LCOW, we already know that IEM cost reduction is necessary in future developments.

Although EDC demonstrate possibility of being competitive to MVC+C, MD+C always requires the highest LCOW among the four technologies investigated. In the average operating scenarios, the LCOW of MD+C is $\$40.32/m^3$, which is $\$28.21/m^3$ higher than EDC and $\$29.53/m^3$ higher than MVC+C. In the optimistic operating scenarios, MD+C is over 200% higher than the next expensive technology. MD+C's high LCOW is due to primary energy consumption (i.e., the electricity necessary for operating the MD module). As such, it can be concluded that MD+C is not an economically competitive technology when using electrical resistive heating. EDC, when compared with MD+C, is a better alternative ZLD desalination technology to MVC+C. However, it is worth noting that if all electricity costs for heating were replaced with free waste heat and the additional infrastructural costs are considered, the LCOW of the average MD+C w/ WH system is decreased to only $\$5.38/m^3$ over that of MVC+C. The MVC+C w/ WH system, however, also shows large variation between operating scenarios. Similarly to the MD+C system, the high energy requirements of the MD module necessitate large waste heat collection and delivery infrastructure. As the energy demand of the system increases, these equipment costs grow as well. Resultingly, the economic competitiveness of the MD+C w/ WH system relies on the optimal energy efficiency of the MD module.

Furthermore, we performed comparative TEA for scenarios where the feedwater consisted of NaCl (see Section Appendix:S.4.4.2.1 of the SI). Compared to the scenarios where the feedwater is consisted of Na_2SO_4, the LCOW of EDC increases significantly (e.g., from $\$12.11/m^3$ to $\$26.90/m^3$ for the average operating scenario, Table S45 and Table S55 in the SI). Because comparisons were made on the basis of consistent feedwater mass concentration (i.e., the NaCl and Na_2SO_4 solutions had the same salt concentration in units of 68,500 ppm in the average scenarios), the much lower molar mass of NaCl ($58.44\ g/mol$) compared to Na_2SO_4 ($142.02\ g/mol$) results in more ions that need to be migrated through the IEMs in EDC. It is worth noting that the additional consideration of the dissociation number of NaCl (2) and Na_2SO_4 (3) returns that NaCl ion concentrations will be 62% higher than those of Na_2SO_4 at any given equal mass-based concentration. Furthermore, experimental results have shown that due to water transportation through the membranes with sodium chloride result in a limiting concentration below that of the saturation limit. As such, no experimental crystallization of sodium chloride has been achieved. This work ignored all water transport within modelling but still shows limitations with sodium chloride crystallization due to the ion concentrations. With improved IEM design, these limitations may be overcome.

The higher ion concentration of NaCl solutions translates to a larger area of IEM needed for EDC operation, which, as discussed above, is a significant cost contributor. However, even with higher LCOW compared to Na_2SO_4 crystallization, EDC still has lower LCOW for NaCl crystallization than MVC+C under the optimistic scenarios. EDC capital costs for NaCl feedwaters are reduced by 79% from the average to the optimistic operating scenarios while MVC+C only experiences a 14% reduction. As with the Na_2SO_4 solutions, most EDC cost savings for NaCl solutions in the optimistic scenario is due to lowered necessary IEM area and lowered IEM costs.

Although the LCOW of MVC+C also increases for NaCl crystallization (e.g., from \$10.79/m^3 to \$12.43/m^3 for the average scenario, Table S45 and Table S55 in the SI), the salt type has less effect on the MVC+C system. As explained above, EDC is sensitive to salt type because its operation is defined by the movement of salt ions through membranes. MD, MVC, crystallizers, RO, and most other desal technologies rely on the removal/movement of water and are, thus, less affected by the type of brine being treated when a consistent volume of water is present.

Though we have learned much from scenario analysis, the local sensitivity assessment can tell us additional operating parameters to specifically focus research on for productive EDC development.

4.3.2. LCOW Local Sensitivity: IEM costs determine EDC competitiveness

A local sensitivity assessment was conducted to determine the effects of specific modelling input parameters on the LCOW of different ZLD technologies. As such, each input variable listed in Table 6 was increased by ±10%, and the respective percentage change of LCOW was calculated. In the current study, only variables that change LCOW by at least 2% are considered significant and graphically represented. Figure 14 shows the sensitivity of LCOW with respect to changes in variables for Na_2SO_4 crystallization. Sensitivity results of LCOW to all input variables are shared in Table S46 through Table S49 of the SI.

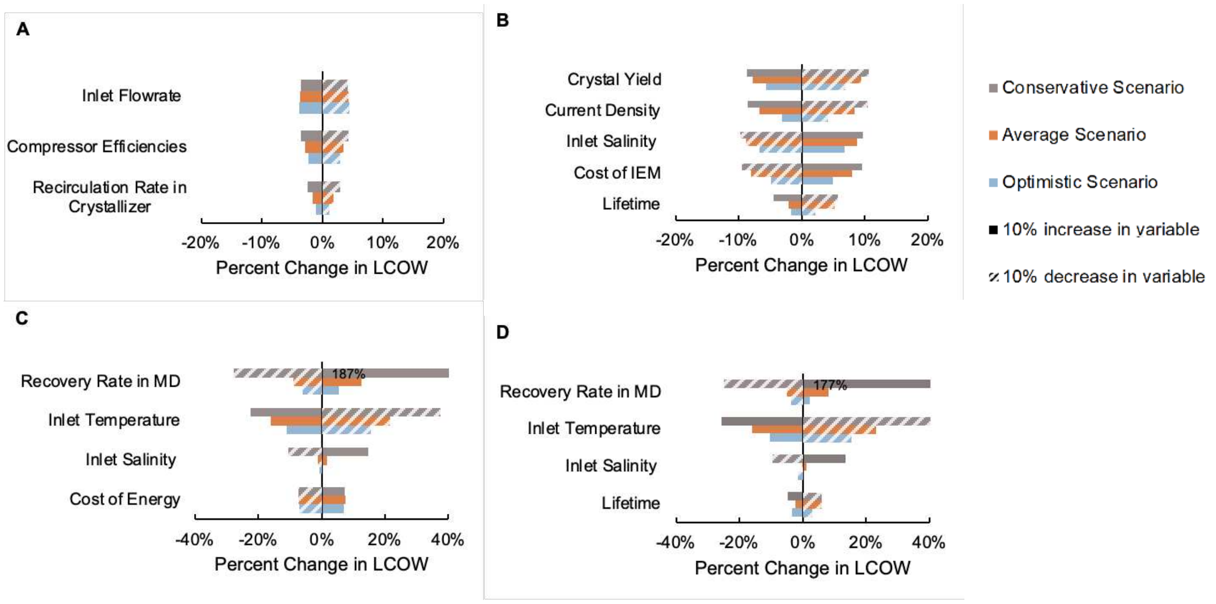

Figure 14: Sensitivity of Levelized Cost of Water Treatment With a 10% Change of Inputs for Na_2SO_4 Crystallization. A) mechanical vapor compression with a crystallizer (MVC+C), B) electrodialytic crystallization (EDC), C) membrane distillation with a crystallizer (MD+C), D) MD+C when using waste heat (MD+C w/ WH). A distinction has been made between increases and decreases to variables in the figure, which demonstrate either a positive (solid bar to the right) or a negative (dashed bar to the right) correlation with cost.

Figure 14A shows that MVC+C is relatively not cost sensitive. The low sensitivity of LCOW to operating parameters for MVC+C is mainly due to the fact that its performance is largely consistent across scale. For example, an increase of flowrate by 10% results in roughly a 5% decrease in LCOW. A higher flowrate will translate to a larger size of the brine treatment system, subsequently taking advantage of economies of scale. Also, increasing the compressor efficiency decreases both capital and operational costs, as a smaller compressor is needed to complete the necessary work and/or less electricity is being consumed. Lastly, increased recirculation rates in the crystallizer result in lower costs, as more thermal energy is conserved in the crystallizer system and less energy supplied by the compressor is needed to induce evaporation.

As shown in Figure 14B, LCOW sensitivity of EDC is much higher than that of MVC+C. EDC LCOW is most sensitive to four parameters including crystal yield, current density, inlet salinity, and the cost of IEMs. The first three parameters are directly correlated to the necessary IEM area for brine crystallization and the increased costs can be traced back to the increase in membrane area. The high sensitivity of EDC LCOW to the cost of IEM necessitates decreasing the cost of IEM to the highest importance for reducing the LCOW of EDC. Such a result explains the variation in comparison between EDC and MVC+C as shown in Figure 13. For example, the higher LCOW of EDC over that of MVC+C in the conservative scenario (Figure 13C) is due to the changes of all parameters at the same time, result in a compounding increase of cost related to the IEM. Lower IEM costs would result in decreased costs and would also decrease the sensitivity of LCOW to parameters such as crystal yield, current density, and inlet salinity. Finally, because of the high capital expenses of the EDC system compared to operational expenses, the lifetime also largely affects the LCOW of EDC. Lifetime has less effect on systems which have lower capital costs in comparison to their operational expenses such as MVC+C and MD+C.

For the MD+C system, LCOW is the most sensitive to MD inlet temperature. The effect of inlet temperature is known to have a large impact on the performance of MD [5, 23, 41, 84]. Specifically, with higher inlet temperatures, MD has lower SEC and a lower necessary membrane area because there is a higher potential for water flux at higher temperature differentials across the membrane. Therefore, as the inlet temperature increases for MD, both capital and operational expenses will decrease, leading to a negative correlation of inlet temperature with LCOW of the MD+C system. An increase of the water recovery rate in the MD system results in higher LCOW, as the MD module has higher SEC than the crystallizer. The increased electricity consumption leads to higher energy costs and, subsequently, LCOW. Finally, because the MD+C system consumes high amounts of electricity, an increase of the cost of electricity also has a large effect on the LCOW.

Figure 14D shows MD+C w/ WH, predictably, has similar sensitivities to MD+C. Though the costs do not track through the same areas, major costs in both the MD+C and MD+C w/ WH systems stem from energy demands of the MD module. As such, the same sensitivities to performance are seen for both technologies. However, MD+C w/ WH is not sensitive to electricity costs. Rather, as with the EDC system, lifetime of the system is an important variable due to the higher ratio of capital expenses stemming from waste heat collection and delivery infrastructure.

The local sensitivity assessments of the four ZLD desalination systems show that no one conclusion on the future direction of desalination can be made for all ZLD technologies. EDC displays the necessity for reduction in membrane cost and future research in economic IEM creation will be paramount to EDC's economic competitiveness. The economic competitiveness of MD+C relies on general MD module performance, as MD has a very high SEC compared to other technologies. MVC+C is a technology with low sensitivity in comparison to the other ZLD systems. This stability makes MVC+C a more predictable technology and reinforces its standing as the baseline ZLD technology to date.

4.3.3. LCA impacts are low for EDC due to low electricity consumption

In this work, LCA was used to quantify the TRACI impacts of each of the four ZLD technologies (i.e., MVC+C, EDC, MD+C, and MD+C w/ WH), in three operating scenarios. The impacts were levelized against the functional unit (i.e., per cubic meter of clean water produced) for reporting. The levelized impacts for the four ZLD technologies operating in the average scenario for Na_2SO_4 crystallization is shown graphically in Figure 15.

Results for NaCl can be found in the Section Appendix:S.4.4.2.2 of the SI. From Figure 15, we see that MVC+C w/ WH has the lowest environmental impact when compared to the other ZLD technologies. EDC has the next lowest impacts, except in ozone depletion. EDC has high ozone depletion in comparison to the other technologies due to the RO and IEM membrane production emitting trichloro-trifluoroethane (CFC113). Over 99% of the contributions to ozone depletion from EDC can be traced to the production of membranes. Overall, this ozone depletion value is not concerning to us. Though the ratio of ozone depletion compared to the other technologies is high, this is more an attribute of how small these impacts are for MVC+C and MD+C, rather than high for EDC. Furthermore, RO is a mature and widely used technology [49]. Because RO is the state-of-the-art desalination technology in low-salinity applications, we believe that the ozone depletion value should not be concerning, as the markets have already shown wide acceptance of this impact.

In all categories but ozone depletion, impacts trend with the consumption of energy (i.e., the SEC of the technology), meaning that in general, lower impacts are associated with technologies that use less electricity. Chemical use shows to have little impact on results due to the low volumes being used. These results show how important reducing electricity consumption is for reducing environmental impacts of desalination technologies. Because the SEC of EDC is lower than either MVC+C or MD+C, its environmental impacts are generally lower. However, because the primary technology of the MD+C w/ WH system does not consume any electricity, its environmental impacts are particularly low.

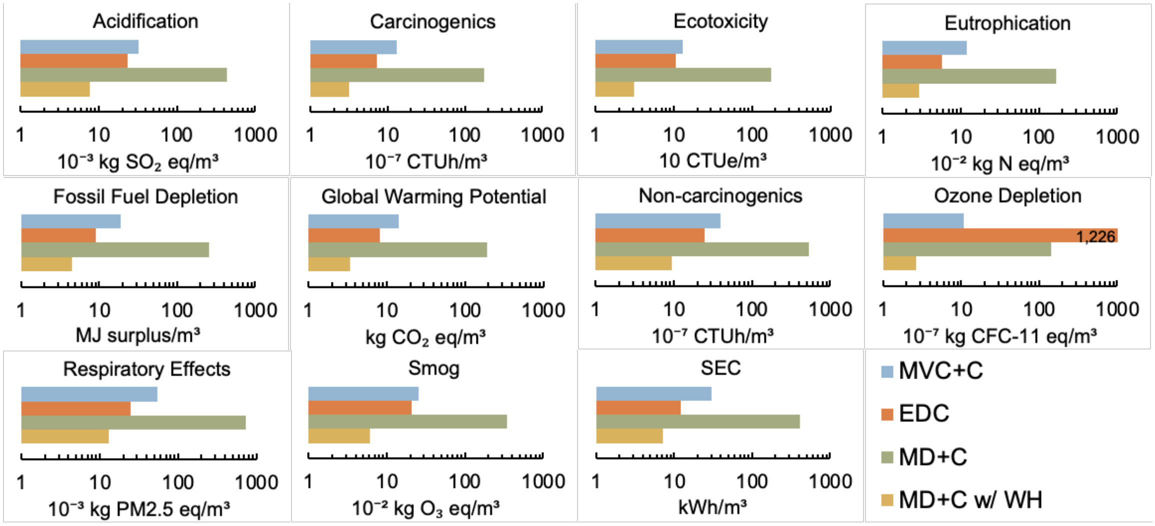

Figure 15: Impacts per Cubic Meter of Treated Water for Na_2SO_4 Crystallization. Results are shown for the average scenario. Included with the TRACI impacts are the specific energy consumption (SEC) of each technology. The trends of most emissions match those of the SEC of technologies, which shows that energy consumption is the most important performance indicator to reduce in order to reduce environmental impacts of technologies. However, in the case of Ozone depletion, electrodialytic crystallization (EDC) shows the highest impact per cubic meter of treated water at roughly 120 milligrams of CFC-11 equivalent per cubic meter. This value is elevated due to the high emission of ethane from the ion exchange and reverse osmosis membranes utilized by the EDC zero liquid discharge desalination system. Mechanical vapor compression paired with a crystallizer (MVC+C), membrane distillation paired with a crystallizer (MD+C), and MD+C when using waste heat (MD+C w/ WH) are the other technologies compared.

MD+C is consistently an order of magnitude higher in impacts than MVC+C, the baseline ZLD technology. Again, MD has very high electricity consumption, and therefore, has a very large emissions impact compared to MVC+C and EDC. Comparatively, MD+C w/ WH, which consumes electricity only through the crystallizer, consumes roughly a third of the electricity and emits roughly a third the emissions of the MVC+C system.

EDC is competitive with existing ZLD technologies when comparing environmental impacts. However, EDC is less competitive with capital costs, and therefore, LCOW. This exemplifies the importance of considering both economic and environmental viability of technologies to inform future development.

4.3.4. GWP Local Sensitivity: Environmental impacts of EDC are predictable

The sensitivity of model inputs on GWP was evaluated using local sensitivity assessment for all four technologies in each of the three operating scenarios. Figure 16 shows the results of the sensitivity assessment for Na_2SO_4 crystallization, where inputs from Table 6 were increased by ±10%. The figure shares only the variables that result in at least a 2% change in GWP. Sensitivity results of GWP to all input variables are shared in Table S51 through Table S54 of the SI.

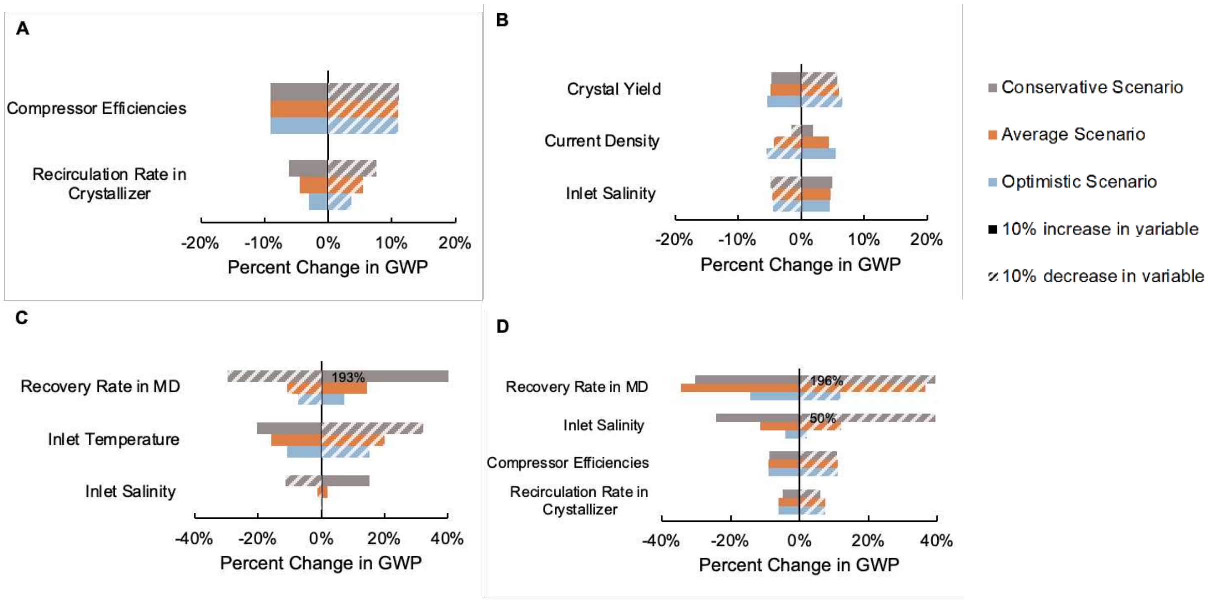

Figure 16: Sensitivity of levelized global warming potential with a 10% change of inputs when removing Na_2SO_4. A) mechanical vapor compression with a crystallizer (MVC+C), B) electrodialytic crystallization (EDC), C) membrane distillation with a crystallizer (MD+C), D) MD+C when using waste heat (MD+C w/ WH). A distinction has been made between increases and decreases to variables in the figure, which demonstrate either a positive (solid bar to the right) or a negative (dashed bar to the right) correlation with global warming potential (GWP).

Figure 16A shows that MVC+C inputs can have a relatively high impact on GWP. As GWP is correlated with SEC (Figure 15), it can be concluded that these variables impact electricity consumption, which makes particular sense for compressor efficiencies. A -9% and +11% change to GWP is seen with a ±10% change to compressor efficiencies. As the compressors are the main consumer of electricity in the MVC+C unit (i.e., pump electricity consumption is negligible), this electricity consumption and GWP change are direct results of efficiency changes. Decreases to the recirculation rate in the crystallizer result in higher electricity consumption. This is due to there being less mass in the system, making temperature changes larger with constant energy depletions, and resulting in higher necessary temperature raises by the compressor. As such, the compressor must work harder to provide enough energy for sufficient heating of the incoming brine. Again, this GWP change can be directly traced to changes in electricity consumption.

As for EDC (Figure 16B), the crystal yield, current density, and inlet salinity are all important in determining electricity consumption, and resulting GWP, of the EDC system. Increased crystal yield results in decreased electricity consumption. Crystal yield can be thought of as the efficiency of the ED system, so it makes sense that an increasing crystal yield results in decreased GWP. In application, crystal yield is largely effected by parasitic water transport across IEMs. As such, improvements to membrane performance would improve the attainable crystal yield of the EDC system and overall environmental results. Current density affects the amount of energy being applied to the system, and increased current density will increase the overall electricity consumption. As expected, an increased salinity will also result in high electricity consumption and GWP, due to the additional ions that need transferred in the system.

MD+C emissions are the most sensitive of the four ZLD systems (Figure 16C). MD+C is most sensitive to recovery rate, inlet temperature, and inlet salinity. As with cost, this a result of the sensitivity to electricity consumption that MD has. Additionally, MD+C has generally higher electricity consumption, and even small changes in percentage scale are translated to be huge overall GWP impacts.

Notably, MD+C w/ WH has opposite reactions to changes in recovery rate and inlet salinity to the MD+C system. Electricity consumption of the MD module drives MD+C environmental impacts. However, electricity consumption is from the crystallizer in the MD+C w/ WH system. As such, the efficiency of the MD module determines MD+C energy consumption, but the efficiency of the crystallizer determines MD+C w/ WH energy consumption. As the performance of the MD module increases, the salinity of the incoming brine to the crystallizer increases. As such, on a levelized basis, the crystallizer consumes more energy when the MD module has higher performance. So, while decreasing recovery rate decreases energy consumption of the MD module, it raises the energy consumption of the crystallizer. A similar effect is had for changes to the inlet salinity. The MD+C w/ WH system has environmental sensitivities to compressor efficiencies and recirculation rate of the crystallizer, because the electricity (i.e., the contributor to environmental impacts) is primarily consumed in the crystallizer.

Overall, EDC shows to have lower environmental sensitivity than the baseline ZLD technology of MVC+C. The environmental sensitivity of MD+C is very high, a result of thermal inefficiencies within the MD unit. That is, due to high sensitivity of energy requirements to changes in input states within the MD unit, high sensitivity of environmental effects are carried through from the impacts of electricity consumption.

4.3.5. LCOW and GWP Tradeoffs

Changes to ED current density showed to have a tradeoff between LCOW and GWP. Increased current density results in the increase of GWP but decreases LCOW. Lower LCOW is a result of the decreased membrane area with increasing current density, but there is a tradeoff with the electricity consumption and environmental impacts. Additionally, the higher LCOW associated with decreasing current density is due to the high costs of IEMs. If IEM costs were to decrease, the optimal current density that balances the tradeoff between

EDC's economic and environmental objectives would decrease, and lower current density would result in better EDC viability. Overall, the EDC system has little inputs that result in competing objectives. With further considerations, identifying the importance of economic and environmental impacts in relation to each other will allow the system to be designed for an optimal current density.

Other tradeoffs exist within the MD+C w/ WH ZLD system. There is a significant tradeoff to any variable which largely impacts the performance (i.e., energy consumption or salt recovery rate) of the MD module. The variables include the recovery rate and inlet salinity of the system. As performance of the MD module increases, LCOW of the system decreases. LCOW is dominated by cost of waste heat collection infrastructure. As such, when the MD module requires less energy, the waste heat collection and delivery technology can be smaller and less expensive. However, this also results in an increase to the levelized electricity consumption of the crystallizer, which increases environmental impacts. Unlike in the MD+C system, a balance must be found between economic and environmental performance when selecting MD+C w/ WH operating parameters.

4.4. Conclusions

Comparative TEA and LCA were conducted to determine the economic and environmental competitiveness of EDC compared to the baseline ZLD desalination technology of MVC+C. Additionally, MD+C and MD+C w/ WH were evaluated for comparisons to a thermal-membrane technology which is also emerging in the concentrated brine desalination market. From the results, it has been shown that the EDC costs (i.e., the LCOW) are competitive with existing ZLD technologies (Figure 13A). There is potential for drastic price reductions, with appropriate focus in future work on reducing the cost of IEMs

(Figure 13B, Section 4.3.1). Furthermore, EDC LCOW has shown to be very sensitive to IEM costs, both directly and secondarily through performance parameters which result in changing membrane area requirements.

Both MD+C costs and environmental impacts are not competitive with either MVC+C or EDC, as MD electricity consumption is very high and results in high costs and environmental impacts. Significant environmental impact reductions are realized when waste heat is utilized in the MD+C w/ WH technology. However, the cost savings are not as drastic for the MD+C w/ WH system in comparison to the MD+C system due to the additional cost of the waste heat collection and delivery equipment cost. With decreased electricity consumption in the MD+C w/ WH technology, environmental impacts are reduced to a level where they compete with EDC and MVC+C as a ZLD application. Costs, however, are less reliable in their ability to compete with the MVC+C ZLD system (Figure 13).

EDC's economic an environmental competitiveness also depends on the salt type being removed. EDC has better performance when crystallizing Na_2SO_4, rather than NaCl. This is due to the ionic concentration of the salts in comparison to their mass concentrations (i.e., their molecular weights and dissociation numbers). As EDC operates by transporting ions across the membrane, the ionic concentration of salts is very important to both the electricity consumption and the size of the EDC system. When crystallizing NaCl, EDC is not cost competitive with existing technologies and is barely competitive in terms of environmental impacts (Table S60 in the SI). When crystallizing Na2SO4, EDC is cost competitive and improves upon the environmental impacts when compared to MVC+C, which makes the technology a good consideration in the paper and textile industries [149, 150]. Further consideration of ED performance should be had when considering application in the electricity production industry, as there is a dual presence of chloride and sulfate ions, which has the potential to significantly reduce the effectiveness of the EDC system, as seen by our results for NaCl removal [151, 152]. Choosing competitive EDC applications will rely highly on the salt being removed from brines.

5. ASSESSING TRIPLE BOTTOM LINE TRADEOFFS OF PRODUCED WATER DESALINATION TECHNOLOGIES IN OIL AND GAS INDUSTRIES

5.1. Overview

5.1.1. Interdisciplinary Considerations

The problem that this work attempts to address, the management of produced waters from the oil and gas industry, is characteristically interdisciplinary. In addition to impacts on local energy and water use, both surface discharge and injection impact communities surrounding waste management sites; by contaminating land, water, and air, through increased noise, and through increased earthquakes due to induced seismicity. These impacts, and others, must be considered when determining whether there are benefits of oil and gas development on both local and global scales. Therefore, a well-defined process and quantitative methodology for assessing the impacts of produced water treatment technologies is greatly needed. Oil and gas wastewater management practices are a noticeable and impactful part of oil and gas development. A short, and by no means comprehensive, list of relevant disciplines that could be leveraged in addressing the problem of produced water management include engineering, sociology, economics, policy, natural resources, and ecosystems management. This work attempts to expand tools available in the technical decision-making processes to consider economic, environmental, and social impacts of produced water desalination.

5.1.2. System Thinking Considerations

This work is strongly motivated by addressing produced water management through a systems-thinking perspective. Technical considerations from previous publications are augmented in this work to include the potential for stakeholder preference considerations and to examine the sensitivity of decision results to said stakeholder preference. The expansion of technical modelling to include economic, environmental, and social models is a result of the systems-thinking approaches being applied in this work.

5.1.3. Stakeholder Engagement

Though this work extrapolates stakeholder opinions through evaluation of digital correspondence (i.e., blogs) and journal publications, there was no direct involvement of either oil and gas or produced water desalination stakeholders beyond the authors listed.

5.1.4. Context of The Drivers, Pressures, States, Impacts and Responses Framework

The Drivers, Pressures, States, Impacts, and Responses (DPSIR) Framework provides integral methodology to this work [153]. First, the DPSIR Framework is used in this work to organize trends from public correspondence and journal publications to supply a simplified, yet comprehensive, list of system considerations affecting Colorado oil and gas development from multiple stakeholder perspectives. Then, the DPSIR Framework is used to create a list of targeted sustainability indicators for the system.

5.1.5. Intellectual Merit and Broader Impacts

In conclusion, the purpose of this research is to broaden the understanding of sustainable operations in ZLD desalination. Sustainability, in the context of this work, is looked upon through the lens of the triple bottom line (TBL) framework, which separates sustainability into economic, environmental, and social indicators. By achieving high performance in each of these three areas, equitable, bearable, and viable system operations can be attained. This chapter, through the EH-DPSIR framework, has begun to define the broader system of ZLD desalination, which will help determine relevant TBL indicators for analysis of these systems. This work has begun assessments of TBL indicators for various ZLD desalination technologies and will be very useful for further sustainability assessments in the oil and gas industry. Results from future variations of this work will be an accumulation of performance in system cost, environmental emissions, and other indicators from all three areas of economic, environmental, and social indicators in one analysis. Furthermore, the methodologies used in this work can be applied to other technologies and industries to broaden the understanding of technology sustainability through system cost and environmental emissions in general. This work will be a helpful tool to stakeholders making decisions surrounding produced water management.

5.2. Introduction

Oil and gas development uses large quantities of water for hydraulic fracturing processes and produces large volumes of wastewaters in the form of produced water (PW). In the Denver-Julesburg Basin of Colorado, wells have been shown to consume over 50,000 cubic meters of water for hydraulic fracturing, and to generate nearly 20,000 cubic meters of PW within the first few months of the production phase [7, 84]. The PW contains high salt contents and, as described in the preceding chapters, requires energy and capital to mitigate environmental impacts it may have.

Oil and gas development is often located near residences and places of public gathering, such as schools, and is an unfortunate result of high-density populations residing over and near areas of high oil and gas production. Previous research has considered management of produced water [16, 19, 23, 25, 47, 51, 68, 83, 84, 154, 155]. Publications have also identified concern in the governance of the oil and gas industry, and the vulnerability of some stakeholders in oil and gas systems [156-158]. However, because the management of oil and gas industry affects the health and safety of so many stakeholders, it is important to consider the social sustainability of oil and gas systems in conjunction with their technical performance. Though there have been publications proposing solutions to technical problems in oil and gas produced water management, and publications on social problems and barriers in oil and gas, there has not been a study that proposes technical solutions to produced water desalination that considers the additional environmental and social barriers that exist within the oil and gas industrial system. This chapter outlines a framework which can be applied to consider the economic, environmental, and social tradeoffs of proposed produced water desalination technologies in the oil and gas industry. The consideration of these three impact areas (i.e., economic, environmental, and social) are defined as the TBL considerations.

Concept mapping and modeling have been used in ecosystems research to understand the relationships between stakeholders, policies, environments, and more within a system [159]. The use of concept mapping in research has been demonstrated as a useful methodology to identify indicators of system performance, guide decision tools, and provide context to complicated multidisciplinary and wicked problems[160-162].

The DPSIR framework was first developed by the European Environmental Agency (EEA) to address the growing need for a standardized systems-thinking approach to the complex and wicked problems facing the modern world [163]. The framework addresses the driving forces of systems, the pressures which complicate their operations, states of systems, impacts that can be made on those systems, and responses that stakeholders make due to those impacts, which then produce additional drivers and pressures within the system. By cyclically identifying the various drivers, pressures, states, impacts, and responses of the system in question, the DPSIR framework enables users to methodically expand their view of the systems in question. Every element of the DPSIR framework is considered a system indicator. However, the EEA DPSIR framework is limited in that it was designed to showcase only environmental systems to guide policy decisions.

In 2015, the US Environmental Protection Agency (EPA) developed a version of the DPSIR framework, which they call the Eco-Health DPSIR (EH-DPSIR), that allows for additional considerations in human health and well-being by splitting the framework into two tracks: the ecosystem health track and the human health track [162]. The EH-DPSIR attempts to avoid analyzing complex systems through a singular perspective. An additional component of the EPA's EH-DPSIR framework is the well-outlined guide to using the tool [153]. The Driver-Pressure-States-Impacts-Responses categories are well-defined and have multiple sub-categories that make the results of using the EH-DPSIR framework consistent across users. The EH-DPSIR framework is being used in this work to bring appreciation to the vast effects that oil and gas wastewater management could have on TBL impacts in an organized and structured way.

Using the EH-DPSIR systems-thinking framework, this work organizes stakeholder perspectives and preferences from literature into a quantifiable TBL impact assessment tool. In this work, a text-frequency methodology is used to identify important considerations for stakeholders which are organized into the EH-DPSIR framework [164, 165]. The EH-DPSIR framework is then used to create a list of prioritized performance indicators that represent social, environmental, and economic considerations for the oil and gas industry in Colorado, which can be used in future works to identify the sustainability of desalination technologies in the oil and gas industry. These indicators can be sourced in a variety of methods from the EH-DPSIR. In most cases, and in the case of this work, all variables found within the EH-DPSIR framework are considered to be indicators [166-173]. In this chapter, technical TEA and LCA results from Chapter 4 are used to demonstrate the potential of this broad consideration of TBL indicators though a scenario assessment of stakeholder preferences.

5.3. Methodology

The graphical abstract of this work is in Figure 17, and outlines the process of taking stakeholder inputs through a EH-DPSIR framework to produce both indicators and provide insight on importance preferences to inform TBL assessments of technology options.

5.3.1. Assessing Stakeholder Perspectives

5.3.1.1. Sourcing Stakeholder Literature

This work analyzes texts from two major stakeholder groups: community members, and researchers. The communities surrounding oil and gas development in the Denver-Julesburg Basin have formed multiple coalitions and alliances to share their opinions on the operation and expansion of oil and gas processes. Specifically, the Larimer Alliance, CRED, Weld Air and Water, Colorado Rising have organized and shared newsletters, blog posts, and forums surrounding oil and gas development. Of these groups, only one has an opinion of approval toward oil and gas development in Colorado: CRED. From the four community sources, 201 documents were created, 38 of which are from CRED. This may bias results toward a critical stance of oil and gas development. However, it may be indicative of community preference for restricting oil and gas development. Each document consisted of a single blog post or update. As there is a larger proportion of critical opinions of oil and gas development based on the sources used, it is important to keep the minority opinion collected for this analysis in view.

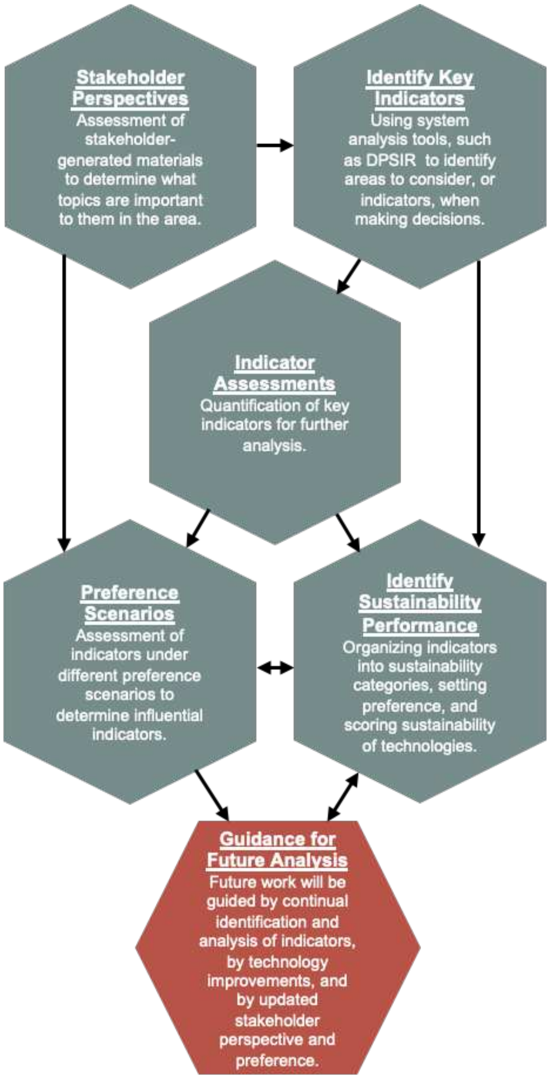

Figure 17: A graphical abstract: This chapter intends to guide future work by distilling important indicators of performance from stakeholder correspondence and publications and framing these indicators though TBL sustainability and stakeholder preference.

Researchers' texts were sourced from peer-reviewed publications. Using the Web-of-Science search tool, "Colorado" and "oil and gas" were searched to be included in any field of texts. 1,980 texts were identified. Metadata of these publications were collected.

Additionally, for further considerations, the additional search-word of "produced water" was included, which narrowed results to 229 texts.

5.3.1.2. Using Stakeholder Literature to Create an EH-DPSIR Framework

There are multiple examples of researchers organizing a DPSIR system from existing literature [164, 165, 167, 174-176]. Methods for identifying DPSIR elements include coding methods, where elements of texts are categorized into "codes" and analyzed once simplified [167, 175]. Other studies began by creating a DPSIR framework and expanded their system based on literature reviews [174, 176].

Some studies use text mining and text frequency (TF) analysis to identify important system considerations [164, 165]. Manservisi et al. [164] used TF-inverse-document-frequency (IDF) methods. Zhou et al. [165] used a TF method. The advantage of an IDF methodology is that it eliminates a single document from over-powering TF calculations, which is possible if there is a particularly long document on a single topic in comparison to the other documents provided. Because the blog posts analyzed were of similar length, an IDF methodology was not deemed necessary. Further consideration may be necessary for future analysis with a broader consideration of texts.

This work uses a TF methodology to analyze the 201 documents, sourced from community publications. The texts were evaluated using the NVivo software package to produce a word frequency analysis. The top 100 words from the documents were also analyzed in a word-associations map within the NVivo software, which connects words which appear together throughout the texts. 10 clusters of words were mapped (Figure S8).

For researchers' texts (i.e., published journal articles), the author-defined keywords were analyzed using TF-methodologies. However, no word-associations were completed for these top words, as they were not found within textual context, but rather listed by authors in an un-related format.

The top 25 words from each source were organized into the EH-DPSIR categories, based on the structured categorizations made by the EPA.

5.3.2. Identification of Key Indicators

Indicators are defined as metrics that can be measured and that help define performative ratings of options within decision analysis [166, 167, 177]. The transition from the DPSIR framework to system TBL indicators is a common practice [166-168]. Though methods for refining the DPSIR system differ, the resulting shift from DPSIR elements to performance indicators is made frequently by finding quantifiable metrics to measure the performance of each DPSIR element; thus, directly making each element of the DPSIR an indicator. Because there is precedence for every element of the DPSIR framework to be an indicator of the system, the key indicators of this work can be directly extracted from the EH-DPSIR created from stakeholder literature.

This work, because it is focused on PW management, first reduced the EH-DPSIR elements by their relevance to PW management. Subsequently, an indicator was given to each EH-DPSI element (responses were not considered as indicators of the system), and possible metrics to quantify performance of said indicators were determined. Finally, it was considered whether each indicator could be accurately represented with the data readily accessible to it from Chapter 4. This process, and notes on it can be seen in Table S68.

5.3.3. Key Indicator Assessments in Technical Scenarios

Chapter 4 presents technological data for four desalination technologies, MVC+C, EDC, MD+C, and MD+C w/ WH, in three technical performance scenarios (conservative, average[7], and optimistic). As such, there are 12 technical scenarios being evaluated in this work. Scores were given to each of the 12 technical scenarios throughout this analysis.

Multiple steps are required to quantify indicator performance for each technical scenario. First, each indicator was quantified using the proposed metrics. Data for each metric is collected to provide a quantification of performance. However, a problem arises when comparing the values of metrics with mis-matching units: it is hard to conceptualize the relative performance of each metric and/or indicator of the system. The solution is to standardize each metric value to a normalized score[61, 171, 178-185]. In this work, each metric is scored from 0-10, with the highest performance being given a 10, and the lowest performance being given a 0. It is a unique coincidence that in this analysis, all metrics have better performance with lower values. As such, the minimum value recorded for a metric is given a score of 10, and the maximum value recorded for a metric is scored a 0. As such, all other metric scores can be determined through a linear scale from 0 to 10, using their metric values, as shown in Equation 20,

$$M_{t,m} = 10 - 10 * \frac{V_{\mathrm{t,m}} - V_{\mathrm{min,m}}}{V_{\mathrm{max,m}} - V_{\mathrm{min,m}}} \tag{20}$$

where $M_{\mathrm{t,m}}$ is the metric score of the m^{th} metric for the t^{th} technical scenario, $V_{\mathrm{t,m}}$ is the metric value of the m^{th} metric for the t^{th} technology scenario, and $V_{\mathrm{min,m}}$and $V_{\mathrm{max,m}}$ are the minimum and maximum metric values of the m^{th} metric across all technical scenarios, respectively.

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[7] Note that average technical scenarios are defined in equivalent ways to Chapter 4. As such, the average scenarios are not a calculated mean of other scenarios considered, but rather an expected performance for each technology.

Because there are multiple metrics to represent a single indicator, metric scores were further combined to an indicator score from 0 to 10. This allows for the comparison of indicators in later steps. Indicator scores were calculated as the average of all relevant metric scores, as shown in Equation 21,

$$I_{t,i} = \frac{\sum M_{t,i}}{N_i} \tag{21}$$

where $I_{\mathrm{t,i}}$ is the i^{th} indicator score for the t^{th} technical scenario, $M_{\mathrm{t,i}}$ are metric scores for the t^{th} technical scenario associated with the i^{th} indicator, and N_{i} is the total number of metrics associated with the i^{th} indicator.

Once indicator scores are obtained for each technology, they are aggregated into TBL scores by categorizing them as either economically, environmentally, or socially focused. TBL scores are the average of the relevant indicator scores, as shown in Equation22,

$$TBL_{t,tbl} = \frac{\sum I_{t,tbl}}{N_{tbl}} \tag{22}$$

where $TBL_{\mathrm{t,tbl}}$ is the TBL score for the t^{th} technical scenario in the tbl category, $I_{\mathrm{t,tbl}}$ are indicator scores for the t^{th} technical scenario associated with the tbl category, and N_{tbl} is the total number of indicators associated with the tbl category.

5.3.4. Technology Assessments in Preference Scenarios

Technology overall scores, or technology preference scores, are determined by further considering the preference of TBL categories and taking weighted averages of TBL scores using importance factors. In similar works, preferences have been based on direct stakeholder feedback [179, 186]. In this work, we choose to provide preference scenarios that allow us to capture a wide range of possible preferences, which has also been represented within literature [61, 178, 185, 187]. Many methodologies have been used to represent preferences in numerous fields [61, 178, 180-184]. Because we have not directly interacted with stakeholders in this analysis, it is best to provide a variety of preference scenarios to provide broad considerations of preferences.

There are 10 scenarios of TBL category preference evaluated in this work, which either prioritize or negate the importance of each TBL category. As such, the preference scenarios are as follows: Only Economic, Only Environmental, Only Social, Equally Weighted, Economically Important, Environmentally Important, Socially Important, Economically Negligible, Environmentally Negligible, and Socially Negligible.

In each preference scenario, an importance factor is assigned to each TBL category. The value of the category's importance factor in relation to the other two TBL categories' determines the weighting of that category in the technology preference scores. Importance factors for each preference scenario considered in this analysis are shared in Table 7. Equation 23 shares the relationship between a technology's TBL scores ($TBL_{t,tbl}$), importance factors ($F_{tbl,p}$), and the technology's overall scores ($P_{t,p}$) for each preference scenario, p.

$$P_{t,p} = \frac{TBL_{t,econ} * F_{econ,p} + TBL_{t,env} * F_{env,p} + TBL_{t,soc} * F_{soc,p}}{F_{econ,p} + F_{env,p} + F_{soc,p}} \tag{23}$$

Table 7: Triple Bottom Line Indicator Preference Scenarios

		Preference Scenario									
		Only Economics	Only Environment	Only Social	Equal Weighting	Economically Important	Economically Negligible	Environmentally Important	Environmentally Negligible	Socially Important	Socially Negligible
Importance Factors (F)	**Economics**	1	0	0	1	3	0	1	2	1	2
	Environment	0	1	0	1	1	2	3	0	1	2
	Society	0	0	1	1	1	2	1	2	3	0

5.4. Results

5.4.1. Extracting Stakeholder Keywords

The top 25 words from this analysis are summarized (Figure 18) and in the Supporting Information in Table S65. Table S65 provides additional context to the 50 (25 from each stakeholder group) stakeholder keywords and justifications for modifications to these keywords that allow for a sharp and succinct representation of the stakeholder views. For example, stakeholder keywords of *fracking*, *fracturing*, and *hydraulic* are combined into the single modified keyword of *hydraulic fracturing*. As another example, additional context is given to the community keyword of *stating*: *stating* and *many* are branched closely to *governments*, *laws,* and *available* (Figure S8). These associated words indicate that, in majority, the use of the words *state, stating, states*, etc. are synonymized with *said*, rather than a physical state of being.

By expanding to the top 100 community keywords and adding on a cluster analysis of these words (Figure S8), a broader understanding of community concerns can be distilled. For instance, *takings* is clustered with *claims* and *property*, which could indicate concern from the community that their property rights are not being respected. Similarly, the cluster of *emissions* and *responsibility* indicate the perceived accountability from the community to sensibly manage emissions. The words from cluster 10 (*page, monitors, reports, air, quality, energy*; Figure S8) show that communities are interested in gaining access to web*pages* that share *air quality* and *energy* data from the oil and gas system. From these considerations, we can conclude that the focus of community is placed on public voice, communication, regulations, and accountability.

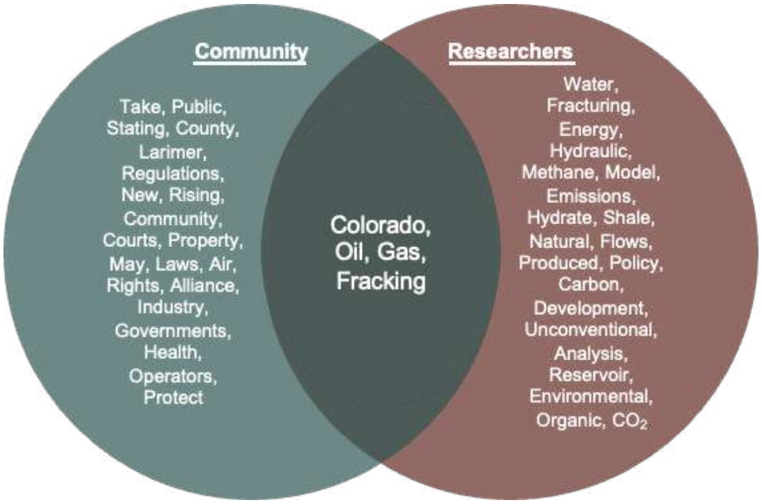

Figure 18: Top 25 keywords from each stakeholder group.

Comparatively, the top 25 keywords distilled from the researcher-identified-keywords of the 1,980 journal articles collected are notably different from those of the community (Figure 18). Of the top words, only a few are similar (i.e., *Colorado*, *oil*, *gas*, and *fracking*). Additionally, these similar words do not add much context to the analysis, as *fracking* processes of the *oil* and *gas* industry in *Colorado* are necessary attributes of the system being considered. Therefore, researchers and community show to have very different perspectives of the system beyond its most basic function.

Researchers seem to be more concerned with emissions, resource flows, and modeling of chemical processes. Additional context to these keywords is provided in the Supporting Information in Table S65. Notably, however, researchers do put importance on *policy*, which appears to be a shared interest with the community stakeholders.

It is also worth noting that economic considerations are not prioritized highly by either shareholder groups. There is a stronger preference for environmental health (*methane, emissions, carbon, environment, VOCs*) and community well-being (*public, regulation, community, property, rights, health, protect*) from the researcher and community stakeholders' perspectives, respectively.

5.4.2. EH-DPSIR

Using distilled stakeholder perspectives from the sources collected and analyzed through the NVivo software, the most important system indicators can be organized into an EH-DPSIR framework. Using a collection of the top 25 words from each perspective, the words are organized into the respective components of the EPA's EH-DPSIR framework. Word clusters (Figure S8) were extensively used at this point to narrow the specificity of the top 25 words from the community stakeholders. The EH-DPSIR organization gives a better understanding of the oil and gas extraction system. The 50 keywords resulted in 172 identified EH-DPSIR sub-elements relevant to produced water management, which are listed in Table S66. A PW-relevant DPSIR element was generated for each. Identification of the PW-relevant DPSIR element allowed for addition context to be communicated about the PW management system. Again, the word clusters from Figure S8 were leveraged at this stage to help define intended word definitions. There were 47 PW-relevant elements named (Table S67, Figure 19). The stakeholder keywords which led to each PW-relevant element were mapped (Table S67). Most importantly, *environmental policy* (mapped from 5 community keywords, 5 researcher keywords, and one keyword from both sources), *discharge regulations (C:4, R:3)*, *atmospheric emissions (C:2, R:4)*, *clean water access (C:2, R:4)*, *public health (C:5, B:1)*, *resource management (C:3, R:3)*, and *stakeholder involvement (C:4, R:1, B:1)* are generated from the most stakeholder keywords, and show a broad importance to the system. There are additional elements shared in Figure 19, which were not generated directly from stakeholder keywords. Rather, the noted elements were added to the figure to fill gaps between DPSIR categories. For example, human behavior pressures were added to connect social drivers to the human states identified. Additionally, economic states were added, which were necessary for capturing performance of *economic prosperity* and *access to jobs*.

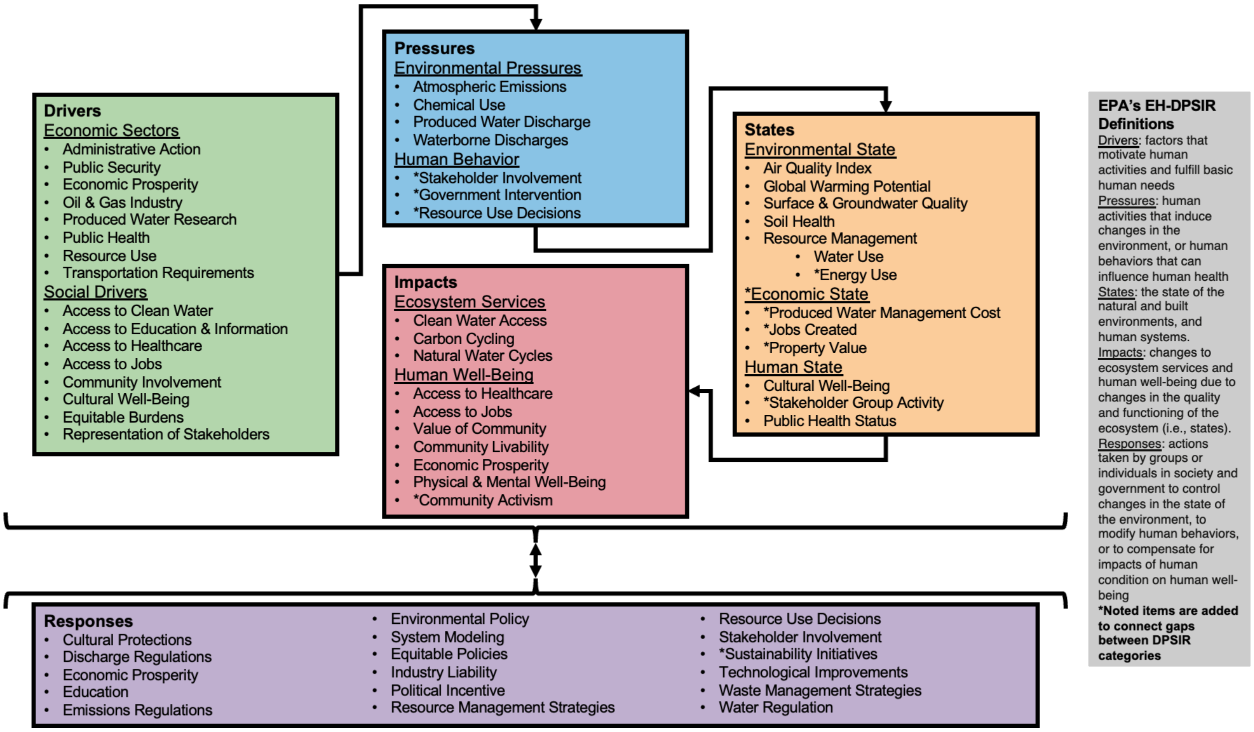

Figure 19: EH-DPSIR generated using keywords distilled from stakeholder literature. Additional author-identified DPSIR elements, denoted with an asterisk, were added to this figure to provide context between the DPSIR categories.

The EH-DPSIR shows that PW management is driven by the need for stakeholder involvement and profitable economic sectors. There are additional pressures surrounding produced water management, including resource management and discharges, that add to the principal goals to be met by a successful system design. Each of these drivers and pressures of the system can be tied to a state, which has a measurable quality to quantifiably define the system. These states include both physical and chemical qualities of ecosystems, economic states, and the health status of communities. The impacts of systems can be identified though the changing of states. Impacts include changes to environmental health, which would be associated with a changing state of measured emissions and chemical discharges. Other impacts could include threats to human wellbeing through decreasing involvement, or inaccessibility to work. The response to these impacts of produced water management may be to change laws and regulations, to increase ecosystem monitoring, or technological innovations. These responses feed back to add additional drivers and pressures on the system (Figure 19).

5.4.3. Key Indicators in Oil and Gas Produced Water Management

All PW-relevant DPSIR elements, excluding the responses of the system, were further considered to provide an indicator for the PW system (Table S66). The 25 identified indicators are listed in Table 8 which also distills the information from Table S66 to link stakeholder keywords to each indicator. The *community livability* indicator appears from the most stakeholder keywords (7 times). *Atmospheric emissions* (6), *public health* (6), *resource management* (6), and *equitable burdens* (5) also show to have broad application to the system. Lastly, metrics were proposed for how to measure each indicator (Table S68). Some indicators use the performance of other indicators as a metric to their performance. For example, *environmental health* is partially measured by *air quality*, which is in turn partially measured by *atmospheric emissions* (Table S68). Subsequently, though not appearing directly from the most modified keywords, *environmental health* results from a large sample of associated stakeholder keywords (12). *Economic prosperity* is a part of *community livability* and is similarly prioritized in this work.

Table 8: Modified keywords that lead to each indicator.

Indicator	Modified Keywords (Stakeholder Source: C=Community, R=Researchers, B=Both)
Access to Clean Water	Water (R)
Access to Education & Information	Community (C), Analysis (R)
Access to Healthcare	Community (C), Health (C)
Access to Jobs	Community (C), Rights (C)
Administrative Action	Court (C), Environment (R), Court (C), Taking (C)
Air Quality	Air (C), VOCs (R)
Atmospheric Emissions	Air (C), Carbon (R), Emissions (R), Industry (C), Methane (R), VOCs (R)
Chemical Use	Industry (C)
Community Involvement	Community (C), Community Organizations (C), Local (B)
Community Livability	Taking (C), May (C), Public (C), Community (C), Government (C), Local (B), Rights (C)
Cultural Well-being	Community (C), May (C), Stating (C), Local (B)
Economic Prosperity	Oil and Gas (B), Community (C), Local (B), May (C)
Environmental Health	Environment (R), Model (R), Property (C)
Equitable Burdens	Government (C), Local (B), May (C), Rights (C), Taking (C)
GHG Emissions	Carbon (R)
Natural Water Cycles	Environment (R), Industry (C), Produced Water (R), Water (R)
Produced Water Discharge	Produced Water (R)
Produced Water Research	Model (R)
Property Value	Property (C)
Public Health	Community (C), Local (B), Air (C), Health (C), Public (C), Rights (C)
Representation of Stakeholders	Taking (C)
Resource Management	Flow (R), Water (R), Industry (C), Produced Water (R), Reservoir (R), Taking (C)
Resource Use	Government (C), Water (R)
Transportation Requirements	Industry (C)
Water Quality	Water (R)

With the indicators having been identified through the EH-DPSIR, the final step was to identify the key indicators for inclusion in this analysis. The justifications for exclusion from or inclusion in this analysis are given for each indicator in the Supporting Information (Table S68). Indicators were excluded due to data availability and for irrelevance when applied to considering different treatment technologies. Those which are included use data generated from Chapter 4 and provide distinctions between technologies. Table 9 summarizes the indicators included in this analysis, and lists the metrics being considered for each. The data used for metric valuation is provided in Table 10. Of the three included key indicators, there is one indicator for each major TBL category: *economic prosperity* as an economic impact, *environmental health* as an environmental impact, and *public health* as a social impact. *Economic prosperity* is represented with TEA results of capital and operational costs from Chapter 4. Though Chapter 4 also supplies data for lifetime costs, they are not included as it would result in the opportunity to double-count technology costs in economic impacts. As such, capital and operational costs are used instead of lifetime costs to increase granularity within the analysis. *Environmental health* and *public health* are represented using LCA results of TRACI impacts for reach technical scenario. *Environmental health* is measured with each of the TRACI impacts generated through LCA methodology. *Public health* is distilled from the human health TRACI impacts: carcinogenics, non-carcinogenics, and respiratory effects (also often called particulates) [143]. Not only are these three key indicators quantifiable from existing data, they are also some of the most frequently identified indicators from stakeholder keywords, which confirms their importance and supports the representation of the PW management system with these three indicators (Table 8, Table S68).

Table 9: Indicators evaluated, and the metrics used to quantify them.

Indicator	Metrics Used
Public Health	• Carcinogenics • Non-carcinogenics • Respiratory Effects
Economic Prosperity	• Capital Costs • Operational Costs
Environmental Health	• Acidification • Carcinogenics • Ecotoxicity • Eutrophication • Fossil Fuel Depletion • Global Warming Potential • Non-carcinogenics • Ozone Depletion • Respiratory Effects • Smog

Table 10: Metric values used to provide metric scores. Sourced from Chapter 4.

Metric (Data Units)	**Cons. MVC+C**	**Avg. MVC+C**	**Opt. MVC+C**	**Cons. EDC**	**Avg. EDC**	**Opt. EDC**	**Cons MD+C**	**Avg. MD+C**	**Opt. MD+C**	**Cons MD+C w/ WH**	**Avg. MD+C w/ WH**	**Opt. MD+C w/ WH**
Acidification (10^{-3} kg SO_2 eq/m^3)	54	45	39	35	33	30	1207	439	261	10	15	17
Carcinogenics (10^{-7} CTUh/m^3)	22	18	16	12	11	10	490	178	106	4	6	7
Ecotoxicity (10 CTUe/m^3)	22	18	16	15	15	13	484	176	105	4	6	7
Eutrophication (10^{-2} kg N eq/m^3)	20	17	15	10	10	8	460	168	100	4	6	6
Fossil Fuel Depletion (MJ surplus/m^3)	32	26	23	16	15	13	714	260	155	6	9	10
Global Warming Potential (kg CO_2 eq/m^3)	24	20	17	17	13	11	542	197	117	5	6	8
Non-carcinogenics (10^{-7} CTUh/m^3)	66	55	48	39	37	33	1482	539	321	12	18	21
Ozone Depletion (10^{-7} kg CFC-11 eq/m^3)	18	15	13	6815	1799	814	402	146	87	3	5	6
Respiratory Effects (10^{-3} kg PM2.5 eq/m^3)	91	75	66	43	42	35	2068	753	447	17	25	29
Smog (10^{-2} kg O_3 eq/m^3)	43	35	31	30	29	26	954	347	206	8	12	13
Levelized Capital Costs (\$/m^3)	9.49	7.90	6.82	131.33	20.39	4.18	31.44	9.06	4.72	50.70	14.56	7.52
Levelized Operating Costs (S/m^3)	6.02	4.53	3.46	27.05	6.52	2.52	108.40	33.09	15.93	7.62	3.45	2.36

5.4.4. Water Treatment Technology Performance Across Indicators

Scores were calculated of each indicator metric based on their metric values (Table S69, Figure 20). In the tabulated form, it is easy to see that the minimum score for most metrics was set by the conservative MD+C technical scenario, except in capital expenses and ozone depletion, which are set by the conservative EDC technical scenario. Discussion on the metric values is made in Chapter 4. MD+C is largely outperformed by MVC+C (Figure 20). Furthermore, MD+C has high variance to its metric scores. The optimistic MD+C technical scenario largely out-scores the conservative MD+C technical scenario. Overall, MD+C's metric scores indicate, even before preference scenarios are considered, that MD+C will not be a competitive option for PW management due to its wide possibility of scores. However, results are much more consistent, and high, for the MD+C w/ WH technology. Apart from capital costs in the conservative and average technical scenarios, MD+C w/ WH performs at largely the same level as MVC+C.

EDC shows more consistency between technical performance scenarios. Scores compete with those of MVC+C in all cases except in ozone depletion and the economic prosperity metrics (Figure 20). However, in the optimistic technical performance scenario, EDC does score equally to MVC+C in all economic prosperity metrics. MVC+C has no variance to metric scores between technical performance scenarios, and consistency scores with a value of 10 in all metrics (Figure 20).

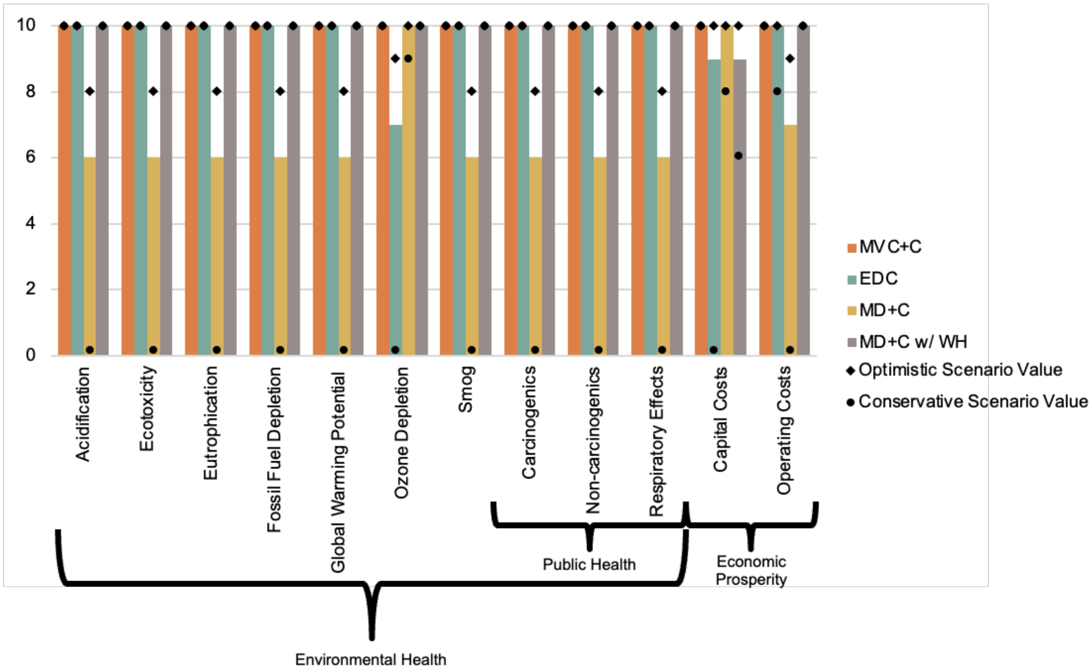

Figure 20: Graphical representation of the scores for each metric in the 12 technical performance scenarios. These values represent the quantitative performance of the technologies in given metrics. The bars represent the score of the average operating scenarios for each technology. The optimistic performance scenarios, scoring higher, are represented for each technology using a diamond data point and the conservative performance scenarios, scoring lower, are represented with a circular data point. Note that the average performance scenario is not a calculated average of the scenarios, but represents the typical, or expected, performance of the technology.

Indicator scores were calculated by averaging the relevant metric scores (Table S69, Figure 21). The indicator scores are the same as the triple bottom line scores, since there is only one indicator represented for each triple bottom line category. As such, indicator scores will be discussed as triple bottom line scores from here forward.

MD+C shows to have high variance between technical performance scenarios in all triple bottom line scores (Figure 21). EDC has high variance in economic scores and shows to have potential for cost savings in the optimal technical performance scenario but is at risk of complete economic divergence from a competitive technology in the conservative technical performance scenario (Figure 21). Similarly, MD+C w/ WH has economic variance in the conservative technical scenario, but scores do not meet those of the conservative EDC and MD technologies. EDC and MD+C w/ WH environmental and social scores, and all MVC+C triple bottom line scores are consistent, and highly performing.

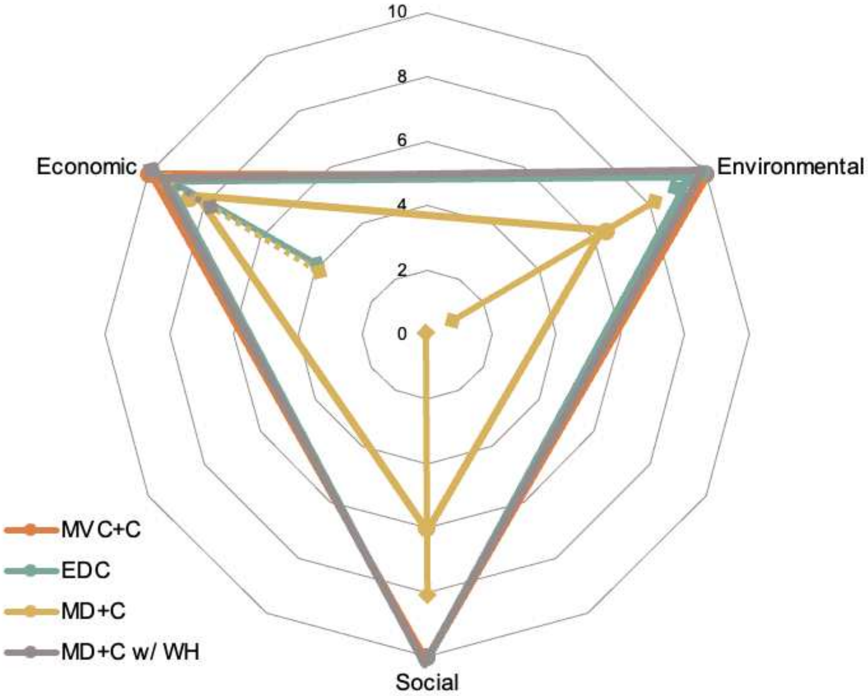

Figure 21: Indicator/triple bottom line scores for technologies operating in the average scenarios. The bars perpendicular to the radial plot lines represent the range of indicator/triple bottom line scores for each technology, stemming from the different technical performance scenarios. There is notable range to the indicator/triple bottom line scores for the MD+C technology in all triple bottom line categories. EDC and MD+C w/ WH also show range to their indicator/triple bottom line scores in the economic category.

5.4.5. Importance Scenario Analysis and Trade-offs of Indicators

Technology preference results were calculated based on TBL importance factors and indicator performances (Figure 22, Table S70). There are no clear TBL tradeoffs for MVC+C and MD+C technologies. MD+C consistently under-performs in every TBL preference scenario when compared to MVC+C. Though there is high variance to each TBL preference scenario score for MD+C, they are consistent across TBL preference scenarios for each MD+C technology performance scenario. MVC+C has consistently high-scoring performance across TBL preference scenarios, which portrays a sense of certainty and security in the technology as an option for PW management compared to MD+C and EDC.

In contrast to MD+C and MVC+C, EDC and MD+C w/ WH appear to be sensitive to TBL preferences (Figure 22, Table S70). In every TBL preference scenario, the optimistic technical performance scenario is one of the best technology options. However, when looking at the average and conservative technical performance scenarios of EDC, TBL preference scenario results depend on the importance factor weightings of economic and social TBL preference. As there is higher preference to social considerations, EDC's score increases. As economic TBL preference increases, EDC is a less-competitive option. In TBL preference scenarios where economic preference is high and social preference is low (economically important, and socially negligible TBL preference scenarios), EDC overall scores decrease. However, in low-economically-focused, and high-socially-focused preference scenarios (economically negligible, and socially important), it shows higher potential for competing with MVC+C as a PW desalination technology. As such, EDC shows to have the most potential for PW management in a scenario where social performance is highly valued and/or when economic performance is not highly valued. Notably, the stakeholders assessed in this work did not put high preference to economic keywords and there is indication toward an economically negligible, or environmentally or socially important TBL preference, which would encourage more EDC considerations.

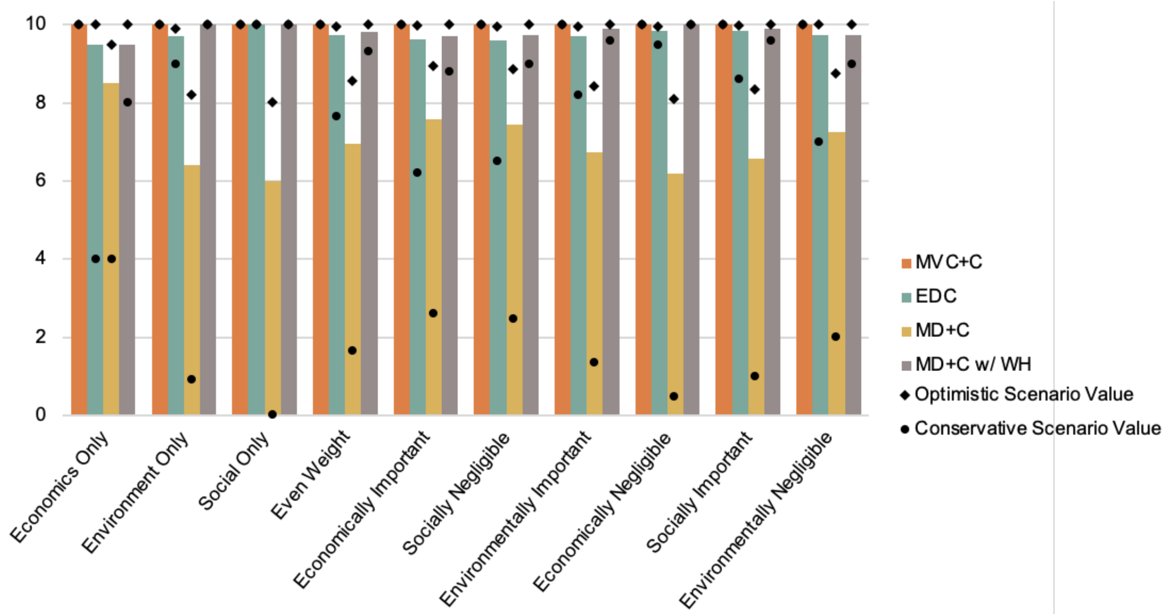

Figure 22: Overall scores from indicator preference scenarios for the 12 technology scenarios. These values represent the qualitative score of technologies when considering different preference weightings. The bars represent the score of the average operating scenarios for each technology. The optimistic performance scenarios, scoring higher, are represented for each technology using a diamond data point and the conservative performance scenarios, scoring lower, are represented with a circular data point. Note that the average performance scenario is not a calculated average of the scenarios, but represents the typical, or expected, performance of the technology.

On a similar note, MD+C w/ WH has sensitivity to economic importance factor weightings. Though it performs well in environmental and social TBL categories, it shows to have inconsistency in economic competitiveness. As such, even though it is still performing at a high level and is near competitive with MVC+C in every option, the preference scenarios with more focus of economic performance (economically important, socially negligible and environmentally negligible) result in lower technology preference to MD+C w/ WH. The competitiveness of MD+C w/ WH relies on the importance of economic performance. In applications of low economic importance, which may be the case for the Colorado oil and gas industry as displayed by stakeholder keywords of this study, MD+C w/ WH is a real option for further consideration.

5.5. Conclusions

This chapter presents assessments of TBL tradeoffs and performance of PW desalination technologies in multiple operating and preference scenarios. Stakeholder generated sources were used to approximate keywords of importance for the stakeholder groups. These stakeholder keywords were expanded using the EH-DPSIR methodology to define indicators of performance within the system. Metrics for measuring the indicator performance were determined and indicators were subsequently scored. Finally, the indicator scores were weighted into an overall technology preference score, based upon TBL indicator preference scenarios.

Review of stakeholder generated materials showed community stakeholders prioritizing community voice and regulations, while researchers prioritize environmentally focused indicators. Both seem to lack a sense of importance to economic considerations. Through the EH-DPSIR framework, stakeholder keywords were expanded to specific elements of the PW desalination system. Each relevant EH-DPSIR element was considered, and an indicator was provided for the assessments made. Each indicator was assigned metrics of performance and measured using data available from Chapter 4. After scoring, results show that MD+C technologies are not capable of out-performing MVC+C, but EDC and MD+C w/ WH have the potential to significantly out-compete MVC+C in environmental and social indicator groups but are sensitive to the preference for economic indicators.

Finally, TBL indicator preference scenarios were analyzed for tradeoffs in scoring. Again, the scores for MVC+C and MD+C were almost equivalent and insensitive to applied preference scenarios. However, EDC and MD+C w/ WH showed a high sensitivity to economic preference in the TBL considerations. In the case of EDC, the low scores from economic importance could be balanced with a higher preference to social performance. For MD+C w/ WH, both environmental and social importance can offset the decrease to overall technology preference scores from poor economic performance. As such, the competitiveness of EDC and MD+C w/ WH are largely determined by the preference for economic indicators, since their competitiveness increases with decreasing economic preference.

In all, results show that MVC+C is a stable and high-performing option for PW management, but EDC and MD+C w/ WH have the potential to compete with MVC+C. As such, future research should be focused on EDC to improve the technical performance and stability of the emerging technology and future research on MD+C w/ WH should focus on improving economic competitiveness. MD+C shows to have low scores in comparison to MVC+C, EDC, and MD+C w/ WH and should not be considered further as an option for PW management.

5.5.1. Limitations of This Chapter and Future Directions in Triple Bottom Line Sustainability Assessments for the Oil and Gas Industry

This chapter shows examples of the additional insights that can be made into technology development when considering TBL indicators, even when partial data inputs are available. In its current state, results from this work can help guide technology development using identified sensitive variables. Specifically, it can be concluded from this work that cost reductions in EDC and MD+C w/ WH technologies will benefit adoption potential. However, at this point, major conclusions on application of technologies to the oil and gas industry in Colorado are largely limited by the lack of:

1) Stakeholder Involvement: The work of this chapter has been completed using limited, publicly available, stakeholder-generated texts. The direct involvement of stakeholders will enrich currently available data and provide further perspectives. Additionally, only community and researcher stakeholder groups were considered. Other stakeholder groups to consider include producers, state-regulators, and local governments. There are largely two direct impacts to this work by limiting stakeholder viewpoints and involvement. First, the system definition (i.e., the completed EH-DPSIR) could be only partially complete. As such, there is a possibility that there are additional indicators than those listed in Table 8. Secondly, limiting of stakeholder perspectives lessens the effectiveness of preference scenarios. Not only could there be scenarios missing from this assessment that no stakeholder would consider as representative of their preference ranking, but the users of this methodology are missing what the frequency of each preference scenario is. For example, if could be that all stakeholders fit within the socially important preference scenario, or they are equally split between environmentally important and economically negligible scenarios. Without a broad consideration of stakeholder preferences, the preference that should be used for decision-making is not known. Additionally, without involving stakeholders to share their direct input of preference, the true preference scenario for the system is not fully understood.

   This limitation can be overcome by:

   a. Creating stakeholder surveys to broaden the definition of the produced water management system in the oil and gas industry in Colorado.

   b. Creating stakeholder surveys that determines the stakeholder-specific importance factors to be used in data-driven preference scenarios.

2) Data Availability: Beyond the limited data from stakeholders, there is also technical data missing from the analysis completed in this work. Not only are there 22 identified indicators that are not considered in this work, there are also multiple metrics missing for each of the three indicators included in this work. All of these omissions are due to data availability at this time. However, these data gaps, once filled, could drastically change the final results of the study. As such, before this methodology, or the results shared within this chapter, are applied to real-world technology application decisions, more indicators (and metrics) should be added to the analysis.

   Future work should focus on making appropriate additions:

   a. Adopt methods for quantifying all indicator metrics identified. In this work, results were limited by data availability, but all indicators should be given the opportunity to be represented within the analysis. Additional data collection or data processing may be needed to consider more indicators in this analysis.

3) Certainty: Due to the amount of data inputs and data processing in the methodology of this analysis, it is difficult to express the certainty of the results calculated. Particularly, once additional technical and stakeholder data are collected, there will be many more inputs and intermediate results considered in this analysis.

There are methods that can be added to this work in future which will help to solidify certainty and reliability of results:

a. Apply statistical methods to capture the uncertainty of these, though methodologically sound, subjectively led and broad analyses of the system. This includes, but is not limited to, a Monte-Carlo analysis.

b. Iterating stakeholder surveys (or interviews, etc.) with data processing and intermediate results development to narrow the preferences of stakeholders throughout the process. The re-visiting of stakeholder inputs throughout the calculations will help to sharpen the understanding of stakeholder perspectives.

c. The use of artificial intelligence software could benefit accuracy of text processing. Particularly, large-language models (LLMs) such as ChatGPT could be leveraged for processing of stakeholder generated materials [188]. The benefit of using LLMs beyond the TF methodology would be in allowing the LLMs to draw conclusions about the intended meanings and contexts of frequent words. Additionally, LLMs could forgo the step of calculating TF, and code themes within text directly, then provide the most coming and most important themes or issues that stakeholders arise. This could be done with existing sources used, and with stakeholder surveys and interview results in future.

6. CONCLUSIONS

6.1. Chapter 3: Viability of Waste Heat Capture, Storage, and Transportation for Decentralized Flowback and Produced Water Treatment

This study provides an in-depth analysis of how waste heat can be collected, stored, and utilized for FPW treatment through membrane distillation using thermodynamic modeling. It examines three scenarios: using waste heat from hydraulic fracturing for on-site treatment, using waste heat from natural gas compressor stations for on-site treatment, and transporting FPW to compressor stations for off-site treatment. The first two scenarios involve addressing mismatches in waste heat availability and FPW treatment demand, requiring storage solutions, while the third compares the costs of transporting FPW versus transporting waste heat to treatment sites.

Key findings indicate that the selection of waste heat storage materials plays a crucial role in determining how much waste heat can be effectively used for treatment. SSMs are less efficient compared to PCMs, which offer advantages through their latent heat properties. TCMs, which maintain constant temperatures, provide even better performance. However, both SSMs and PCMs limit heat utilization due to temperature gaps that make part of the collected waste heat unusable.

The study measures energy consumption in fluctuating conditions using ASEC. Among the materials analyzed, some TCMs prove to be the most effective for enabling complete FPW treatment. Additionally, transporting waste heat, rather than FPW, emerges as a more cost-effective solution, especially when leveraging waste heat from natural gas compressor stations, offering significant potential for transportation cost savings.

The study concludes that decentralized treatment, using stored waste heat from hydraulic fracturing or transported waste heat, is a feasible approach in certain cases. Transporting waste heat, when compared to wastewater transportation, has the potential to considerably reduce costs.

The major conclusions of Chapter 3 are:

1) **Material selection is critical for waste heat utilization**: The type of waste heat storage material significantly impacts the efficiency of FPW treatment using membrane distillation. TCMs, especially those with constant high discharge temperatures, outperform other materials like SSMs and PCMs.
2) **Transporting waste heat is more cost-effective than transporting FPW**: In scenarios where waste heat is transported from natural gas compressor stations, this method proves to be more cost-efficient than transporting the FPW to the treatment site. This can lead to significant savings in transportation costs.
3) **Decentralized treatment is viable under specific conditions**: Both on-site FPW treatment using waste heat from hydraulic fracturing and transported waste heat are feasible when sufficient waste heat is available. Decentralized approaches offer viable alternatives to centralized wastewater treatment systems, particularly when supported by the right storage materials.

6.2. Chapter 4: Targeting Sustainable Desaliantion Solutions: A Techno-economic and Life Cycle Approach to Guiding Zero Liquid Discharge Desalination

The study presents a comparative TEA and LCA to evaluate the economic and environmental competitiveness of EDC in comparison to established ZLD desalination technologies, (i.e., MVC+C). Additionally, MD+C and MD+C w/ WH were assessed as an emerging thermal-membrane technology in the concentrated brine desalination market. The analysis shows that EDC demonstrates competitive LCOW compared to existing ZLD technologies. There is significant potential for further cost reductions in EDC, particularly through future innovations aimed at reducing the cost of IEMs. EDC's LCOW is highly sensitive to the price of IEMs, both in direct costs and through the influence from other performance parameters, which affect the required membrane area.

In contrast, MD+C currently lacks economic competitiveness due to its high electricity consumption, leading to elevated costs and substantial environmental impacts. In the scenario where waste heat could be utilized, MD+C w/ WH may be more viable. Environmental impacts for the MD+C w/ WH system are much lower than the MD+C system. However, costs are still high due to waste heat collection and delivery infrastructure costs replacing those of electricity consumption. The study highlights that the largest contributor to MD+C's (using either electricity or waste heat as an energy source) cost is its energy consumption, so any reduction in energy demand could potentially allow MD+C to compete with technologies like EDC or MVC+C in ZLD applications.

Another important conclusion is that the economic and environmental competitiveness of EDC also depends on the specific salt type being crystallized. EDC performs better when used for the crystallization of sodium sulfate (Na_2SO_4) rather than sodium chloride (NaCl). This is due to differences in ionic concentration, which impacts electricity consumption and the system size for EDC, since the technology operates by transporting ions across membranes. When processing NaCl, EDC is not economically competitive with existing technologies and shows only marginal improvements in environmental impact. However, in the case of Na_2SO_4, EDC becomes both cost-competitive and environmentally advantageous compared to MVC+C, suggesting that its effectiveness is closely tied to the composition of the brine.

The major conclusions of Chapter 4 are:

1) **EDC's economic and environmental performance is highly influenced by the cost and performance of IEMs.** Focusing future research on reducing IEM costs could significantly enhance EDC's overall cost-competitiveness, making it a more attractive alternative to traditional ZLD desalination technologies.
2) **The choice of salt type greatly affects EDC's performance.** EDC showing far better results when processing sodium sulfate compared to sodium chloride. EDC is more cost-effective and environmentally friendly with Na_2SO_4, while its performance with NaCl lags far behind competing technologies. Therefore, careful consideration of the brine composition is essential for choosing suitable EDC applications.
3) **The use of waste heat instead of electricity for treatment using MD does not lower overall system cost.** While the use of waste heat does significantly reduce overall environmental effects due to reduced electricity emissions, the cost of waste heat collection and delivery infrastructure negates economic advantages of using "free" waste heat instead of costly electricity. In general, the high energy demands of MD result in high costs – either from electricity, or from waste heat utilization infrastructure.

6.3. Chapter 5: Assessing Triple Bottom Line Sustainability of Produced Water Desalination Technologies in Oil and Gas Industries

This chapter assessed the tradeoffs and performance of PW desalination technologies by employing a TBL approach, assessing environmental, social, and economic factors. The

EH-DPSIR framework was used to identify key performance indicators that represent various stakeholder interests and system dynamics. Stakeholder-generated sources were critical in identifying areas of importance for each group, which were further expanded upon with relevant indicators. Each indicator was assigned metrics, scored based on available data, and integrated into a final performance score using different TBL preference scenarios.

The results indicated clear differences in stakeholder priorities: community stakeholders emphasized regulations and community representation, while researchers focused more heavily on environmental sustainability. Both groups, however, showed a lack of emphasis on economic considerations, which may influence future technology assessments and adoption. From a technological perspective, MD+C technologies failed to surpass the performance of the state-of-the-art MVC+C system, particularly in terms of overall robustness. EDC and MD+C w/ WH, on the other hand, demonstrated promising potential, competing with MVC+C in social and environmental performance but showing significant sensitivity to economic indicators.

The tradeoff analysis revealed that EDC's competitiveness is highly dependent on how much weight is placed on economic and social factors. When economic considerations were minimized, EDC became more competitive due to its strong environmental performance. However, this also indicates that EDC's viability may vary significantly depending on stakeholder preferences, especially when economic performance is prioritized. Similarly for MD+C w/ WH, low preference to economic performance results in higher system potential. However, MD+C w/ WH's high performance in environmental and social indicators results in less reliance on economic factors than EDC.

Although these results provide valuable insights into desalination technology performance, the limited data restricts the ability to draw definitive conclusions about future technology implementation. As such, no major conclusions are called out from this chapter. Nonetheless, the analysis showcases the value of incorporating TBL indicators and stakeholder preferences into technology assessments, offering a more holistic view of potential trade-offs and benefits.

6.4. Future Work and Recommendations

This work began by evaluating the technical viability of waste heat utilization in the oil and gas industry for produced water desalination using MD (Chapter 3). Then, 4 technology options were modeled, and evaluated for economic and environmental performance (Chapter 4). Finally, this work considered the produced water management system which involved stakeholders, to determine the fit of the 4 technology options into the existing oil and gas industry for produced water desalination (Chapter 5). Continuations on the work completed in this document should include the use of artificial intelligence, increases to model detail, expanding the modeled system boundaries, and involvement of stakeholders. Additionally, because of this work, there are many future research opportunities which do not directly affect the methodologies of this work, but which could direct technological advances in future work. Both improvements and future directions to this research and other research are included in the following sections.

6.4.1. Use of Artificial Intelligence in Future Assessments

- Future iteration of this work should consider the benefits which could be had through utilization of artificial intelligence software. Particularly, LLMs could support the distillation of stakeholder areas of importance and important system indicators from stakeholder generated texts, stakeholder surveys, and stakeholder interviews.

- Artificial intelligence software could also be used to iteratively interface with stakeholders as results of TBL technology preference results are updated to anonymously refine the TBL category importance factors, etc.

6.4.2. Improvements to Technological and System Modeling

- Improved technical models to be based on scale test facilities for EDC and MD systems. Currently, the EDC and MD models are based on bench-scale testing. Subsequently, the models used in this work for EDC and MD may be mis-representing the performance of the technologies at full-scale.
- Future models should expand MD+C w/ WH economic and environmental models to include the storage of waste heat, as explained in Chapter 3. The economic and environmental analysis included in this work only consider the basic technology necessary for transferring heat from one place to another, but does not consider the additional costs of waste heat storage and/or transportation.
- The system modeled should be expanded to include transportation requirements for waste heat, brine, and clean water for all technology options. Particularly when considering membrane distillation systems where waste heat is sourced from off-site locations, transportation can have a large effect on economic and environmental impacts. Furthermore, the social impacts of transportation can be large, as air quality, noise pollution, and traffic are all increased with additional transportation requirements.

- Future analysis should consider clean water valuation opportunities. That is, the value of clean water uses (e.g., reuse in oil and gas extraction activities, discharges to surface, municipal uses, agricultural uses, etc.) can also be evaluated. Economic and environmental credits can be associated with the displacement of other water sources by using the treated produced water product.
- Future assessments should develop methods for quantifying additional indicator metrics. New or adapted methodologies should be explored to ensure that all identified indicators can be accurately quantified, avoiding the limitations of data availability encountered in this work. This may require integrating innovative data collection or modeling techniques to ensure that the analysis captures all necessary aspects of the system. Expanding the scope of data sources and improving data granularity will ensure more reliable and actionable results.
- Application of statistical methods to capture uncertainty in all modeling efforts is needed to reinforce the potential of this work influencing technology application decisions. Implementing statistical tools will allow the analysis to account for inherent uncertainties in both the subjective nature of stakeholder inputs and the broad scope of the system. Techniques such as Monte Carlo simulations or sensitivity analysis could help quantify the impact of uncertain parameters and validate the robustness of the results. These methods will provide greater confidence in conclusions, especially when handling varying preferences and incomplete data.

6.4.3. Stakeholder Involvement in Future Work

- Direct involvement of stakeholders is paramount to accurately defining the produced water management system. Conducting interviews and creating stakeholder surveys to broaden the definition of the produced water management system in the oil and gas industry in Colorado will benefit the system greatly.

- Stakeholders should be directly involved in determining the stakeholder-specific importance factors to be used in creating data-driven preference scenarios.
- Future analysis should also consider stakeholder perspectives beyond those of only the community and researchers. There are many missing stakeholder groups from the work completed in this study, and results can be contextualized in a more representative manner with the additional considerations of industry, local governments, regulating bodies, etc.

6.4.4. Complementary Research Objectives Supported Through This Work

- Bench scale modelling of waste heat storage and utilization by membrane distillation will allow for validation of the modelling done in this work and provide context to the system inefficiencies that will be faced at scale applications.
- The development of low-cost IEMs is paramount to decreasing EDC costs. Not only will the overall costs of the system decrease, but the LCOW will become less sensitive to operating variability, and overall TBL preference of EDC will increase.
- Improving IEM performance should also be focused on. IEMs with increased ion flux, without compromising water flux, would result in lower membrane areas being needed, helping with high membrane costs. Additionally, there is potential for less electricity being needed with better designed membranes. Overall competitiveness of EDC would improve with better IEMs. Furthermore, NaCl crystallization may become competitive, as necessary membrane area decreases.

- Reduction of MD energy requirements is necessary. In either case of MD utilizing waste heat or electricity for heating of brine, the energy intensity of the system necessitates capital or operating costs that are in far excess of existing technologies. Improvements to either, or both, energy recovery measures within the MD system or improved thermal insulative properties of MD membranes could improve costs and raise the potential for MD adoption in the desalination field.

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APPENDIX A: SUPPORTING INFORMATION

S.1. Waste Heat Options and Availability Calculations

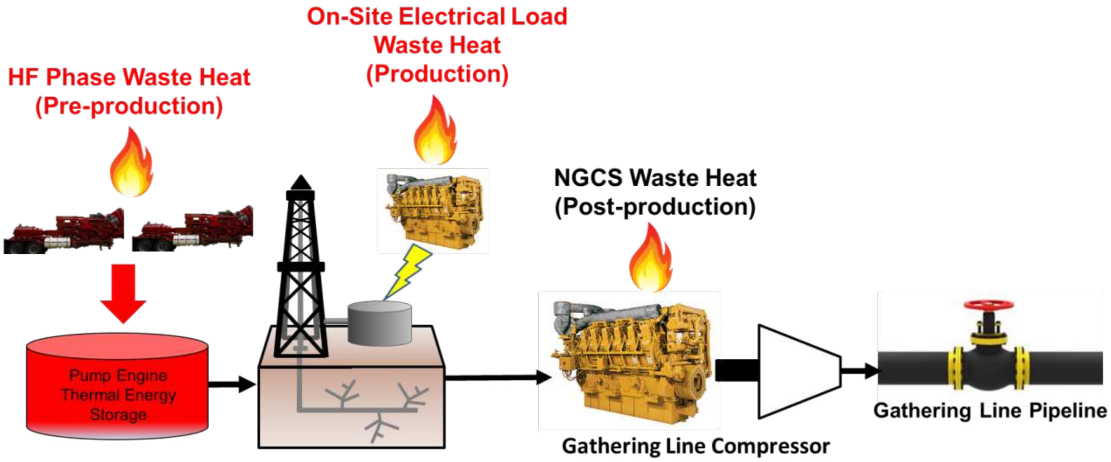

Figure S1. Sources of waste heat available during UOG production process. Waste heat from the HF phase (pre-production) and from the on-site electrical load (production phase) are used for analysis because they are able to power on-site MD treatment of UOG wastewater (highlighted by red).

Table S1. Detailed calculation for waste heat available during HF operation based on theoretical pressures, volumetric flow rates, and operating efficiencies.

Variable	Assumption	Value	Units
Water volume (V_{water})	Typical water volume per well [4]	4.1-22.5×10^6	gal
Initial pressure (P_{i})	Ambient pressure	100	kPa
Pumping pressure (P_{pump})	Typical HF pressure [189]	6000	psi
Pump efficiency (η_{pump})	Typical pump efficiency [86, 88]	89	%
Engine efficiency (η_{eng})	Typical diesel engine efficiency [86]	43	%
Safety factor (SF)	Ensures enough power is provided	1.5	-
HF duration (Δt_{f})	HF pump operational time	16-91	Hours
Waste heat capture efficiency (η_{waste})	Assume 100% capture efficiency to represent highest possible energy content	100	%
Variable	**Equation**	**Value**	**Units**
Required volume flow water ($\dot{V}_{\text{water}}$)	$\dot{V}_{\text{water}} = \frac{V_{\text{water}}}{\Delta T_{\text{f}}}$	0.26	m^3 s^{-1}
Required pressure increase (ΔP)	$\Delta P = P_{\text{pump}} - P_{\text{i}}$	41.3	MPa
Pump power ($\dot{W}_{\text{pump}}$)	$\dot{W}_{\text{pump}} = \dot{V}_{\text{water}} \Delta P * SF$	16.1	MW
Engine power ($\dot{W}_{\text{eng}}$)	$\dot{W}_{\text{eng}} = \frac{\dot{W}_{\text{pump}}}{\eta_{\text{pump}}}$	18.1	MW
Waste heat rate ($\dot{Q}_{\text{waste}}$)	$\dot{Q}_{\text{waste}} = \frac{\dot{W}_{\text{eng}}}{\eta_{\text{eng}}} * (1 - \eta_{\text{eng}})$	24	MW
Total waste heat available (E_{waste})	$E_{\text{waste}} = \dot{Q}_{\text{waste}} \Delta t_{\text{f}} * \eta_{\text{waste}}$	1.4-7.9×10^9	kJ

Table S2. Detailed calculation for waste heat available from on-site electrical loads based on survey of industry standard data sheets.

Variable	Assumption	Value	Units
Waste heat rate ($\dot{Q}_{\text{waste}}$)	Typical waste heat from engine at 50% load delivering 8 to 10 kW of power	18.95	kW
Duration (Δt)	Total operating time	12	Months
Variable	**Equation**	**Value**	**Units**
Total waste heat available (E_{waste})	$E_{\text{waste}} = \dot{Q}_{\text{waste}} \Delta t$	5.9×10^8	kJ

Table S3. Survey of industry standard data sheets (Caterpillar, Cummins, GENERAC, Kohler)

Manufacturer **-**	**Model #** **-**	**Fuel Type** **-**	**Load** **%**	**Power** **kW**	**Fuel Input Power** **kW**	**Thermal Efficiency** **%**	**Coolant Heat** **kW**	**Exhaust Heat** **kW**	**Heat Accounted For** **%**
CAT	DE7.5E3S	Diesel	100	8	31.25	26	10	7.16	81%
CAT	DE9.5E3	Diesel	100	8	32.33	25	10	7.16	78%
CAT	DE9.5E3B	Diesel	100	8	31.25	26	10	7.16	81%
CAT	DE11E3S	Diesel	75	9	35.56	25	10.28	8.19	77%
CAT	DE13.5E3	Diesel	75	9	34.48	26	10.17	8.10	79%
CAT	DE13.5E3B	Diesel	75	9	34.48	26	10.17	8.10	79%
KOHLER	15REOZK	Diesel	75	9.75	43.11	23	14.50	2.40	62%
CAT	DE16E3S	Diesel	50	8.8	35.56	25	10.49	7.49	75%
CAT	DE18E3	Diesel	50	8	33.41	24	8.24	5.78	66%
GENERAC	RD020	Diesel	50	10	39.80	25	9.50	7.34	67%
CUMMINS	C20D6	Diesel	50	9.1	35.89	25	13.55	8.59	87%
GENERAC	SD020	Diesel	50	9	43.11	21	11.47	7.84	66%
KOHLER	20REOZK	Diesel	50	8.25	38.09	22	10.96	14.47	88%
CAT	DE22E3B	Diesel	50	9	35.56	25	10.43	7.45	76%
CAT	DE22E3	Diesel	50	9	35.56	25	10.43	7.45	76%
CUMMINS	C35D6	Diesel	25	8	42.78	19	10.02	9.69	65%
GENERAC	SD035	Diesel	25	8	39.10	20	7.68	9.94	66%
GENERAC	SG035	Gas	25	8	67.32	12	11.16	7.31	39%
CUMMINS	C40D6	Diesel	25	9	47.31	19	10.55	10.85	64%
GENERAC	SD040	Diesel	25	9	42.11	21	8.58	11.33	69%
KOHLER	40REOZK	Diesel	25	8.5	49.12	17	8.90	8.66	53%
KOHLER	KG40	Gas	25	9.25	63.72	15	15.00	14.90	61%
KOHLER	50REOZK	Diesel	25	10	49.12	20	10.00	8.93	59%

S.2. Natural Gas Composition

The composition of natural gas determines its lower heating value (LHV), which represents the amount of thermal energy released from burning/combusting the gas. The composition of natural gas changes significantly throughout regions in the U.S. In order to make a reasonable estimation for the Denver-Julesburg (DJ) Basin, the thermal energy contained in natural gas must be calculated based on the corresponding composition. Once the molecular percentage (*molf*) of each compound is known, the corresponding mass fraction (*mf*) can be calculated using the molecular weight (*MW*). The *mf* is then used to calculate the LHV using Equations S1-S3 as below.

$$MW_i = \sum_i^{elements} MW_{element} * N_{element} \tag{S1}$$

$$mf_i = {molf_i * MW_i}\Big/{\sum_i^n molf_i * MW_i} \tag{S2}$$

$$LHV = \sum_i^n mf_i * LHV_i \tag{S3}$$

Table S4 shows a typical gas composition for the DJ Basin according to the U.S. Geological Survey [92]. Table S5 describes the calculation of LHV for natural gas in the DJ basin based on the composition and compound properties shown in Table S4. Our calculation method resulted in a LHV of 45.8 MJ kg-1 in the DJ Basin. This correlates well with the typical LHV of treated natural gas (44-57 MJ kg-1) [190, 191]. Because the referenced composition has a variety of compounds that account for the remaining 1.7%, the major compounds are normalized to yield a mole fraction sum of 1.

Table S4: Composition of a typical natural gas mixture in the Denver-Julesburg Basin.

Compound	**Composition**		**Compound Properties**			
	Molar Percentage	**Normalized $molf_i$**	**LHV_i (kJ kg^{-1})**	**N_{Carbon}**	**$N_{Hydrogen}$**	**N_{Oxygen}**
Methane	82.6%	0.840	50024	1	4	0
Ethane	10.1%	0.103	47509	2	6	0
Propane	2.7%	0.028	46331	3	8	0
Pentane	0.3%	0.003	45717	5	12	0
Carbon Dioxide	2.6%	0.026	0	1	0	2
Totals	98.3%	1	--	--	--	--

Table S5: Detailed calculation for heat available from burning natural gas.

Variable	**Assumption**	**Value**	**Units**
Molecular Weight CH_4	Chemical formula	16.0	g mol^{-1}
Molecular Weight C_2H_6	Chemical formula	30.1	g mol^{-1}
Molecular Weight C_3H_8	Chemical formula	44.1	g mol^{-1}
Molecular Weight C_5H_{12}	Chemical formula	72.1	g mol^{-1}
Molecular Weight CO_2	Chemical formula	44.0	g mol^{-1}
Variable	**Equation**	**Value**	**Units**
Total Mass per Mole (M)	$M = \sum_i molf_i MW_i$	19.2	g mol^{-1}
Mass Fraction CH_4 (mf_{CH4})	$mf_{CH4} = \frac{molf_{CH4} MW_{CH4}}{M}$	0.70	-
Mass Fraction C_2H_6 (mf_{C2H6})	$mf_{C2H6} = \frac{molf_{C2H6} MW_{C2H6}}{M}$	0.16	-
Mass Fraction C_3H_8 (mf_{C3H8})	$mf_{C3H8} = \frac{molf_{C3H8} MW_{C3H8}}{M}$	0.06	-
Mass Fraction C_5H_{12} (mf_{C5H12})	$mf_{C5H12} = \frac{molf_{C5H12} MW_{C5H12}}{M}$	0.01	-
Mass Fraction CO_2 (mf_{CO2})	$mf_{CO2} = \frac{molf_{CO2} MW_{CO2}}{M}$	0.06	-
Lower Heating Value (LHV)	$LHV = \sum_i mf_i LHV_i$	45.8	MJ kg^{-1}

S.3. Waste Heat Accessibility

S.3.1. Representative Wells and Storage Materials

Table S6: Data on flowback and produced water and waste heat generation for the wells investigated in this study [4]

Well Name	**Well API#**	WH	FPW_{day}
-	-	GJ	m^3/day
Cervi	41222	2053.87	55.8
Dukes Federal	42981	3584.00	111.5
Ehrlich	43541	1997.36	33.1
Hazzard Federal	42980	1642.11	89.1
Hood	44371	2328.68	27.1
Horsetail	41774	2569.61	74.6
J Klein	42999	2741.38	35.2
Jaguar	42622	4036.25	75.7
JZM	42666	3994.56	130.7
Markham	43247	1585.86	123.0
Orr State	43975	2416.89	15.1
Peterson	44718	3057.83	21.5
Puma Fed	42566	2589.44	26.1
RBF	44446	2179.49	26.8
Stromberger	42557	5828.74	12.9
TC Hiland Knolls	43516	3750.09	60.5
Varra	39983	2362.58	289.6
Wells Ranch State	43879	7866.87	65.7
Wilson Ranch	41066	2488.18	42.8
Woolley Sosa	38110	2669.17	57.6

Waste heat values were calculated by assuming each well produces 349.3 kJ of waste heat for every gallon of water that is used during hydraulic fracturing. This assumption considers both pumping and engine efficiencies of 89% and 43%, respectively, and a required pressure increase of 41 MPa for fracturing. These assumptions are used and justified in our previous publication [5].

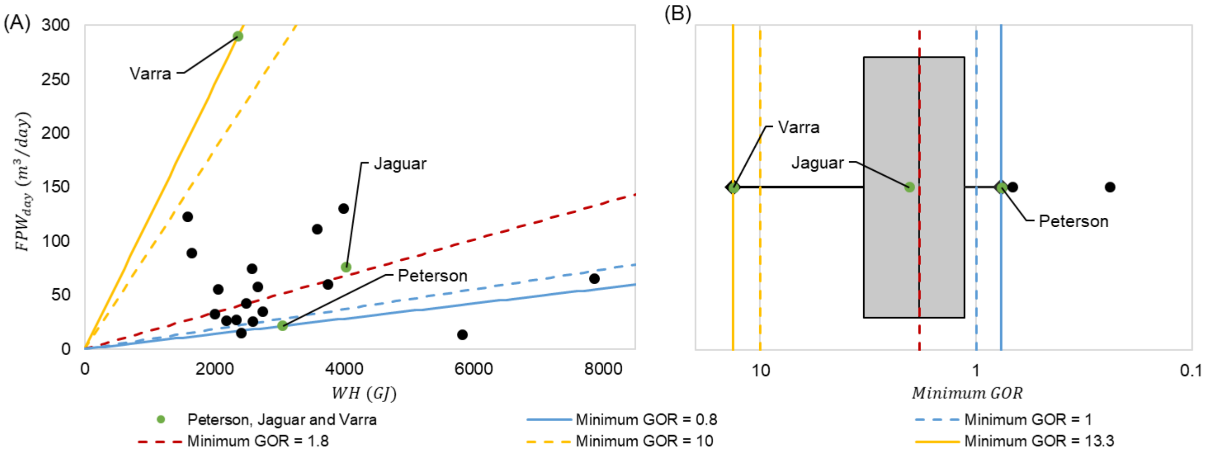

Figure S2: (A) A plot comparing daily flowback and produced water production and total waste heat generation of each well from Table 1. (B) Distribution of the minimum GOR needed for the waste heat availability to meet treatment demands for the same 20 wells. The first quartile value is 0.8, median value is 1.8 and third quartile number is 13.3.

Table S7: Properties of sensible and phase change material for waste heat storage considered in this study

Storage Material	**Type**	ρ	T_{pc}	Δh_{pc}	ΔH	E_{density}	**References**
-	-	kg/m^3	$°C$	kJ/kg	kJ/kg	MJ/m^3	-
Water	SSM	965	-	-	293	283	[100]
Paraffin Wax	PCM	670	56	143	282	189	[192]
n-Pentacosane	PCM	801	54	238	395	317	[193]
n-Hexacozane	PCM	803	56	256	419	336	[193]
n-Heptacozane	PCM	779	59	235	387	301	[193]
n-Nonacozane	PCM	808	63	239	405	327	[194]
n-Triacontane	PCM	775	65	252	410	318	[194]
Myristic Acid	PCM	860	54	190	349	300	[195]
Palmitic Acid	PCM	850	64	185	334	284	[193]
Stearic Acid	PCM	940	69	209	354	333	[196]

Table S8: Thermo-chemical waste heat storage materials that use water as the sorbate

Sorbent	Type	T_{charge}	T_{dis}	E_{density}	References
-	-	$°C$	$°C$	MJ/m^3	-
Lithium Bromide	Liquid Absorbent	81	40	1127	[93, 97, 197]
Lithium Chloride	Liquid Absorbent	66	66*	1440	[93, 197]
Potassium Hydroxide	Liquid Absorbent	63	63*	1127	[93, 197]
Sodium Hydroxide	Liquid Absorbent	98	63	727	[93, 97, 197]
Calcium Sulfate	Chemical Adsorbent	150	89	1400	[94, 198]
Magnesium Chloride	Chemical Adsorbent	130	100	2001	[93, 95, 197]
Magnesium Sulfate	Chemical Adsorbent	150	111	3063	[93-95, 197]
Silica Gel	Solid Physical Adsorbent	88	70	180	[93, 97]
Zeolite 13X	Solid Physical Adsorbent	173	63	547	[93, 97]
Zeolite 13XBF	Solid Physical Adsorbent	150	75	277	[93, 97]
Zeolite 4A	Solid Physical Adsorbent	205	60	384	[93, 97]

Materials with charging temperature above the temperature of available waste heat will result in the material not being charged. The assumption made that all waste heat is available at 90°C makes some of these thermo-chemical storage materials infeasible. However, these materials are still included in this analysis, in the case that waste heat above 90°C is available .

*The discharge temperature for lithium chloride and potassium hydroxide were not provided, and therefore are assumed to be equal to the charging temperature.

S.3.2. Membrane Distillation Treatment Performance

Table S9: The energy consumption and water productivity of direct contact membrane distillation as a function of heat source temperature

Feedwater Temperature $°C$	$\boldsymbol{SEC}$ $\boldsymbol{kJ/kg}$	$\dot{\boldsymbol{m}}_{\mathbf{clean}}$ $\boldsymbol{kg/s}$	$\dot{\boldsymbol{V}}_{\mathbf{treat}}$ $\boldsymbol{m^3/day}$	**Heat Source Temperature ($\boldsymbol{T}$)** $°C$
40	4369	0.001	0.13	40.38
45	3469	0.002	0.20	45.30
50	2850	0.003	0.28	50.31
55	2391	0.004	0.38	55.36
60	2034	0.005	0.51	60.41
65	1750	0.006	0.66	65.46
70	1516	0.008	0.84	70.59
75	1332	0.010	1.04	75.54
80	1174	0.012	1.28	80.59
85	1046	0.015	1.57	85.65
90	940	0.018	1.90	90.71

This table shows values calculated in the DCMD model used for the study. Actual values were calculated for every 0.01°C increment of feedwater temperature. These values represent the properties of a single MD module. The model has been developed and used in our previous publication [5].

S.3.3. Example Calculations for Charging Storage Materials with Collected Waste Heat

Table S10: Charging model example using Jaguar well

Water	**Paraffin Wax**	**Calcium Sulfate**
Equation 4.1		
$N = \frac{75.7\ \mathrm{m}^3/day}{1.90\ \mathrm{m}^3/day} = 39.8 \rightarrow 40$		
Equation 5.1		
$m_{store} = \frac{4036.25 * 10^6\ kJ}{293\ kJ/kg}$ $= 13775\ Mg$	$m_{store} = \frac{4036.25 * 10^6\ kJ}{282\ kJ/kg}$ $= 14312\ Mg$	-
Equation 6.1		
$V_{store} = \frac{4036.25 * 10^6\ kJ}{283\ MJ/m^3}$ $= 14262\ m^3$	$V_{store} = \frac{4036.25 * 10^6\ kJ}{189\ MJ/m^3}$ $= 21356\ m^3$	$V_{store} = \frac{4036.25 * 10^6\ kJ}{1400\ MJ/gallon}$ $= 2883\ m^3$

S.3.4. Consideration of Transportation Weight

Volume of storage materials is important when considering the number of trucks needed to transport waste heat from natural gas compressor stations to wells for treatment. By determining the volumetric treatment capacity of the storage material, we can determine if a lesser volume is transported when decentralized treatment is compared to centralized treatment. Of the storage materials that allow for lower transportation distances (4 found in the main text; magnesium sulfate, magnesium chloride, calcium sulfate, and lithium chloride), we need to now consider their weight. A truck in Colorado is limited to 36.3 metric tons [199]. Comparing this to the limitation we have of 6,000 gallons (22.7 cubic meters) per truck, we know that any material with a maximum density (i.e., a hydrated density, in the case of TCMs), over 1.6 times the destiny of water will need to have additional trucks than determined by the volumetric treatment capacity (Eq. S4).

$$Sg_{lim} = 1.6 = \frac{36300\ kg}{(997\frac{kg}{m^3}*22.7m^3)} \tag{S4}$$

We can also determine the maximum factor that can be applied to each material before transportation of waste heat is no longer a viable option. This is equal to the volumetric treatment capacity of the material (i.e., the inverse of the value calculated in Equation 18 of the main manuscript). This number is recorded in Table S11 as X_{max}. We evaluate magnesium sulfate, magnesium chloride, calcium sulfate, and lithium chloride to determine their hydrated densities using the following methods. The rest of the materials have already been determined as infeasible options due to their volumetric treatment capacities. To determine the hydrated densities of each thermos-chemical material, we use three material properties: the number of water molecules per hydrated sorbent molecule (N_H), the molecular weight of the materials (MW), and their densities (ρ) (Table S11).

Table S11: Additional thermo-chemical waste heat storage material characteristics

Sorbent	N_H	**MW**	ρ	X_{max}	X_W	**Limiting?**	**References**
-	-	kg/mol	kg/m^3	-	-	-	-
Lithium Chloride	1	42.39	2070	1.03	0.98	No	[3]
Calcium Sulfate	2	136.14	2320	1.79	1.13	Yes	[3]
Magnesium Chloride	6	95.21	2320	2.63	0.85	No	[3]
Magnesium Sulfate	7	120.37	2660	4.00	0.90	No	[3]

We determine the mass of water needed per mass of sorbent (k, Eq. S5) and then calculate the hydrated densities (ρ_h, Eq. S6).

$$k = N_H * MW_{water}/MW_{sorbent} \tag{S5}$$

$$\rho_h = [1 + k] * \left[\frac{1}{\rho_{sorbent}} + \frac{k}{\rho_{water}}\right]^{-1} \tag{S6}$$

Once we know the hydrated density of the TCM, we can calculate the hydrated specific gravity of the sorbent (Sg, Eq. S7). Dividing the hydrated specific gravity by 1.6, the limited specific gravity of the material, will return the multiplication factor (X_w, Eq. S8), which we apply in Eq 16 of the main manuscript to find the total number of trucks needed for waste heat transportation.

$$Sg = \rho_h/\rho_{water} \tag{S7}$$

$$X_w = Sg/Sg_{lim} \tag{S8}$$

From Table S11, we see that only Calcium Sulfate is limited further by weight constraints, but it does not reach the maximum factor which would render the transportation of thermo-chemical storage material less economically viable than transportation of FPW.

S.3.5. Supplemental Results for All Wells

Table S12: Jaguar well results from waste heat storage modelling

WH (GJ):	4036.25	MD Modules:	41
FPW_{day} (m^3/day):	75.7	Minimum GOR:	2.03
		Critical SEC (kJ/kg):	1111

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	29 - 38	36 - 60	14260	8.27 - 10.86	1369 - 1743
Paraffin Wax	PCM	17 - 39	20 - 71	21356	11.97 - 28.4	1370 - 2013
n-Pentacosane	PCM	12 - 37	15 - 75	12745	7.57 - 23.68	1373 - 2248
n-Hexacozane	PCM	11 - 39	14 - 75	11993	6.77 - 23.07	1367 - 2136
n-Heptacozane	PCM	11 - 41	14 - 74	13383	7.24 - 25.92	1371 - 2032
n-Nonacozane	PCM	41 - 45	65 - 75	12317	6.02 - 6.57	1747 - 1845
n-Triacontane	PCM	44 - 47	66 - 75	12689	5.93 - 6.41	1682 - 1775
Myristic Acid	PCM	13 - 37	16 - 73	13440	8.01 - 22.79	1378 - 2193
Palmitic Acid	PCM	42 - 46	64 - 74	14200	6.8 - 7.4	1692 - 1792
Stearic Acid	PCM	46 - 50	65 - 74	12125	5.37 - 5.81	1560 - 1664
Lithium Bromide	Liquid Absorbent	25	100	3580	3.18	4483
Lithium Chloride	Liquid Absorbent	64	100	2801	0.97	1743
Potassium Hydroxide	Liquid Absorbent	59	100	3580	1.33	1881
Sodium Hydroxide	Liquid Absorbent	59	100	5547	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	88	2881	0.63	973
Magnesium Chloride	Chemical Adsorbent	100	86	2015	0.44	954
Magnesium Sulfate	Chemical Adsorbent	100	86	1317	0.29	954
Silica Gel	Solid Physical Adsorbent	72	100	22409	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	60	100	7374	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	82	100	14562	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	54	100	10518	4.29	2060

Table S13: Varra well results from waste heat storage modelling

WH (GJ):	2362.58	MD Modules:	157
FPW_{day} (m^3/day):	289.6	Minimum GOR:	13.30
		Critical SEC (kJ/kg):	170

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	5 - 7	41 - 69	8347	7.16 - 9.38	1368 - 1740
Paraffin Wax	PCM	3 - 7	24 - 85	12501	10.07 - 23.8	1368 - 2011
n-Pentacosane	PCM	2 - 6	17 - 86	7460	6.61 - 20.58	1371 - 2245
n-Hexacozane	PCM	2 - 7	16 - 86	7020	5.93 - 20.13	1365 - 2134
n-Heptacozane	PCM	2 - 7	16 - 85	7834	6.3 - 22.46	1369 - 2030
n-Nonacozane	PCM	7 - 8	74 - 86	7210	5.26 - 5.73	1746 - 1844
n-Triacontane	PCM	8 - 8	76 - 86	7427	5.17 - 5.59	1681 - 1774
Myristic Acid	PCM	2 - 6	19 - 84	7867	6.97 - 19.73	1377 - 2190
Palmitic Acid	PCM	7 - 8	74 - 86	8312	5.88 - 6.4	1691 - 1791
Stearic Acid	PCM	8 - 9	74 - 85	7097	4.69 - 5.07	1559 - 1663
Lithium Bromide	Liquid Absorbent	4	100	2095	3.18	4483
Lithium Chloride	Liquid Absorbent	10	100	1640	0.97	1743
Potassium Hydroxide	Liquid Absorbent	9	100	2095	1.33	1881
Sodium Hydroxide	Liquid Absorbent	9	100	3247	2.07	1881
Calcium Sulfate	Chemical Adsorbent	17	100	1686	0.56	973
Magnesium Chloride	Chemical Adsorbent	18	100	1180	0.38	954
Magnesium Sulfate	Chemical Adsorbent	18	100	771	0.25	954
Silica Gel	Solid Physical Adsorbent	11	100	13117	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	9	100	4317	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	13	100	8524	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	8	100	6157	4.29	2060

Table S14: Peterson well results from waste heat storage modelling

WH (GJ):	3057.83	MD Modules:	12
FPW_{day} (m^3/day):	21.5	Minimum GOR:	0.76
		Critical SEC (kJ/kg):	2965

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	58 - 76	27 - 45	10804	10.99 - 14.45	1370 - 1747
Paraffin Wax	PCM	32 - 76	15 - 51	16179	16.6 - 39.58	1370 - 2016
n-Pentacosane	PCM	24 - 76	11 - 57	9656	9.9 - 31.17	1373 - 2250
n-Hexacozane	PCM	23 - 80	11 - 58	9086	8.8 - 30.18	1368 - 2138
n-Heptacozane	PCM	23 - 82	11 - 57	10139	9.54 - 34.29	1371 - 2033
n-Nonacozane	PCM	84 - 92	50 - 57	9331	7.88 - 8.59	1747 - 1846
n-Triacontane	PCM	89 - 96	50 - 57	9613	7.79 - 8.42	1683 - 1776
Myristic Acid	PCM	26 - 75	12 - 55	10182	10.55 - 30.15	1379 - 2196
Palmitic Acid	PCM	85 - 92	48 - 56	10758	9.03 - 9.83	1692 - 1794
Stearic Acid	PCM	94 - 100	49 - 55	9186	7.13 - 7.6	1560 - 1630
Lithium Bromide	Liquid Absorbent	66	100	2712	3.18	4483
Lithium Chloride	Liquid Absorbent	100	59	2122	1.65	1743
Potassium Hydroxide	Liquid Absorbent	100	63	2712	2.10	1881
Sodium Hydroxide	Liquid Absorbent	100	63	4202	3.26	1881
Calcium Sulfate	Chemical Adsorbent	100	33	2183	1.69	973
Magnesium Chloride	Chemical Adsorbent	100	32	1527	1.18	954
Magnesium Sulfate	Chemical Adsorbent	100	32	998	0.77	954
Silica Gel	Solid Physical Adsorbent	100	52	16977	13.17	1541
Zeolite 13X	Solid Physical Adsorbent	100	63	5587	4.33	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	46	11032	8.56	1350
Zeolite 4A	Solid Physical Adsorbent	100	69	7968	6.18	2060

Table S15: Cervi well results from waste heat storage modelling

WH (GJ):	2053.87	MD Modules:	31
FPW_{day} (m^3/day):	55.8	Minimum GOR:	2.95
		Critical SEC (kJ/kg):	767

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	20 - 27	36 - 60	7256	8.18 - 10.73	1369 - 1743
Paraffin Wax	PCM	12 - 27	21 - 72	10867	11.81 - 28.01	1370 - 2013
n-Pentacosane	PCM	8 - 26	15 - 76	6486	7.49 - 23.42	1372 - 2247
n-Hexacozane	PCM	8 - 27	14 - 76	6102	6.69 - 22.83	1367 - 2136
n-Heptacozane	PCM	8 - 28	14 - 75	6810	7.16 - 25.62	1371 - 2031
n-Nonacozane	PCM	29 - 31	66 - 76	6268	5.96 - 6.49	1747 - 1845
n-Triacontane	PCM	30 - 33	67 - 76	6457	5.87 - 6.34	1682 - 1775
Myristic Acid	PCM	9 - 26	16 - 74	6839	7.92 - 22.53	1378 - 2193
Palmitic Acid	PCM	30 - 32	65 - 75	7226	6.72 - 7.32	1692 - 1792
Stearic Acid	PCM	32 - 35	65 - 75	6170	5.31 - 5.74	1560 - 1664
Lithium Bromide	Liquid Absorbent	17	100	1822	3.18	4483
Lithium Chloride	Liquid Absorbent	44	100	1425	0.97	1743
Potassium Hydroxide	Liquid Absorbent	41	100	1822	1.33	1881
Sodium Hydroxide	Liquid Absorbent	41	100	2823	2.07	1881
Calcium Sulfate	Chemical Adsorbent	79	100	1466	0.56	973
Magnesium Chloride	Chemical Adsorbent	80	100	1025	0.38	954
Magnesium Sulfate	Chemical Adsorbent	80	100	670	0.25	954
Silica Gel	Solid Physical Adsorbent	50	100	11403	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	41	100	3752	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	57	100	7410	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	37	100	5352	4.29	2060

Table S16: Dukes Federal well results from waste heat storage modelling

WH ($\boldsymbol{GJ}$):	3584	MD Modules:	61
$\boldsymbol{FPW}_{\textbf{day}}$ ($\boldsymbol{m^3/day}$):	111.5	Minimum GOR:	3.37
		Critical SEC ($\boldsymbol{kJ/kg}$):	670

Storage Material	Type	$\boldsymbol{FPW}_{\textbf{treat}}$	$\boldsymbol{WH}_{\textbf{util}}$	$\boldsymbol{V}_{\textbf{store}}$	Inverse Volumetric Treatment Capacity	$\boldsymbol{ASEC}$
-	-	%	%	$\boldsymbol{m^3}$	$\boldsymbol{m^3/m^3}$	$\boldsymbol{kJ/kg}$
Water	SSM	19 - 24	38 - 63	12663	7.76 - 10.18	1369 - 1742
Paraffin Wax	PCM	11 - 26	22 - 77	18963	11.1 - 26.3	1369 - 2013
n-Pentacosane	PCM	8 - 24	16 - 80	11317	7.13 - 22.27	1372 - 2247
n-Hexacozane	PCM	7 - 25	15 - 80	10649	6.38 - 21.73	1367 - 2136
n-Heptacozane	PCM	7 - 26	15 - 79	11884	6.81 - 24.34	1371 - 2031
n-Nonacozane	PCM	26 - 29	69 - 79	10937	5.67 - 6.18	1746 - 1845
n-Triacontane	PCM	28 - 30	70 - 80	11267	5.59 - 6.03	1682 - 1775
Myristic Acid	PCM	8 - 24	17 - 77	11935	7.54 - 21.4	1378 - 2192
Palmitic Acid	PCM	27 - 30	69 - 79	12609	6.38 - 6.94	1692 - 1792
Stearic Acid	PCM	29 - 32	69 - 79	10766	5.06 - 5.47	1560 - 1663
Lithium Bromide	Liquid Absorbent	15	100	3179	3.18	4483
Lithium Chloride	Liquid Absorbent	38	100	2487	0.97	1743
Potassium Hydroxide	Liquid Absorbent	36	100	3179	1.33	1881
Sodium Hydroxide	Liquid Absorbent	36	100	4925	2.07	1881
Calcium Sulfate	Chemical Adsorbent	69	100	2558	0.56	973
Magnesium Chloride	Chemical Adsorbent	70	100	1789	0.38	954
Magnesium Sulfate	Chemical Adsorbent	70	100	1169	0.25	954
Silica Gel	Solid Physical Adsorbent	43	100	19898	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	36	100	6548	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	50	100	12930	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	33	100	9339	4.29	2060

Table S17: Ehrlich well results from waste heat storage modelling

WH ($\boldsymbol{GJ}$):	1997.36	MD Modules:	18
$\boldsymbol{FPW}_{\textbf{day}}$ ($\boldsymbol{m^3/day}$):	33.1	Minimum GOR:	1.80
		Critical SEC ($\boldsymbol{kJ/kg}$):	1259

Storage Material	Type	$\boldsymbol{FPW}_{\textbf{treat}}$	$\boldsymbol{WH}_{\textbf{util}}$	$\boldsymbol{V}_{\textbf{store}}$	Inverse Volumetric Treatment Capacity	$\boldsymbol{ASEC}$
-	-	%	%	$\boldsymbol{m^3}$	$\boldsymbol{m^3/m^3}$	$\boldsymbol{kJ/kg}$
Water	SSM	30 - 39	32 - 54	7057	9.08 - 11.93	1369 - 1744
Paraffin Wax	PCM	17 - 40	18 - 64	10568	13.34 - 31.72	1370 - 2014
n-Pentacosane	PCM	12 - 38	13 - 69	6307	8.26 - 25.9	1373 - 2249
n-Hexacozane	PCM	12 - 41	13 - 69	5935	7.37 - 25.18	1367 - 2137
n-Heptacozane	PCM	12 - 42	13 - 68	6623	7.92 - 28.4	1371 - 2032
n-Nonacozane	PCM	43 - 47	59 - 69	6095	6.57 - 7.17	1747 - 1846
n-Triacontane	PCM	45 - 49	60 - 69	6279	6.49 - 7.01	1682 - 1775
Myristic Acid	PCM	13 - 38	15 - 67	6651	8.76 - 24.98	1378 - 2194
Palmitic Acid	PCM	44 - 47	59 - 68	7027	7.46 - 8.12	1692 - 1793
Stearic Acid	PCM	48 - 52	59 - 68	6000	5.86 - 6.34	1560 - 1664
Lithium Bromide	Liquid Absorbent	28	100	1771	3.18	4483
Lithium Chloride	Liquid Absorbent	72	100	1386	0.97	1743
Potassium Hydroxide	Liquid Absorbent	67	100	1771	1.33	1881
Sodium Hydroxide	Liquid Absorbent	67	100	2745	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	77	1426	0.72	973
Magnesium Chloride	Chemical Adsorbent	100	76	997	0.50	954
Magnesium Sulfate	Chemical Adsorbent	100	76	652	0.33	954
Silica Gel	Solid Physical Adsorbent	82	100	11089	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	68	100	3649	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	93	100	7206	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	61	100	5205	4.29	2060

Table S18: Hazzard well results from waste heat storage modelling

WH (GJ):	1642.11	MD Modules:	49
FPW_{day} (m^3/day):	89.1	Minimum GOR:	5.89
		Critical SEC (kJ/kg):	384

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	11 - 14	39 - 65	5802	7.61 - 9.98	1369 - 1741
Paraffin Wax	PCM	6 - 15	23 - 79	8689	10.84 - 25.68	1369 - 2012
n-Pentacosane	PCM	4 - 14	16 - 81	5185	7 - 21.85	1372 - 2246
n-Hexacozane	PCM	4 - 15	15 - 81	4879	6.27 - 21.34	1367 - 2135
n-Heptacozane	PCM	4 - 15	15 - 81	5445	6.68 - 23.86	1371 - 2031
n-Nonacozane	PCM	15 - 17	70 - 81	5011	5.57 - 6.07	1746 - 1845
n-Triacontane	PCM	16 - 18	71 - 81	5162	5.48 - 5.92	1682 - 1774
Myristic Acid	PCM	5 - 14	17 - 79	5468	7.4 - 20.99	1378 - 2192
Palmitic Acid	PCM	16 - 17	70 - 81	5777	6.26 - 6.81	1691 - 1792
Stearic Acid	PCM	17 - 19	70 - 80	4933	4.97 - 5.37	1559 - 1663
Lithium Bromide	Liquid Absorbent	9	100	1456	3.18	4483
Lithium Chloride	Liquid Absorbent	22	100	1140	0.97	1743
Potassium Hydroxide	Liquid Absorbent	20	100	1456	1.33	1881
Sodium Hydroxide	Liquid Absorbent	20	100	2257	2.07	1881
Calcium Sulfate	Chemical Adsorbent	39	100	1172	0.56	973
Magnesium Chloride	Chemical Adsorbent	40	100	820	0.38	954
Magnesium Sulfate	Chemical Adsorbent	40	100	536	0.25	954
Silica Gel	Solid Physical Adsorbent	25	100	9117	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	21	100	3000	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	28	100	5924	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	19	100	4279	4.29	2060

Table S19: Hood well results from waste heat storage modelling

WH (GJ):	2328.68	MD Modules:	15
FPW_{day} (m^3/day):	27.1	Minimum GOR:	1.26
		Critical SEC (kJ/kg):	1788

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	40 - 52	30 - 51	8227	9.74 - 12.79	1370 - 1745
Paraffin Wax	PCM	22 - 52	17 - 59	12321	14.46 - 34.42	1370 - 2015
n-Pentacosane	PCM	16 - 51	13 - 64	7354	8.83 - 27.72	1373 - 2249
n-Hexacozane	PCM	16 - 54	12 - 65	6919	7.86 - 26.9	1368 - 2137
n-Heptacozane	PCM	16 - 56	12 - 64	7721	8.48 - 30.43	1371 - 2033
n-Nonacozane	PCM	57 - 62	56 - 64	7106	7.02 - 7.66	1747 - 1846
n-Triacontane	PCM	60 - 65	56 - 64	7321	6.93 - 7.49	1682 - 1776
Myristic Acid	PCM	18 - 51	14 - 62	7754	9.38 - 26.76	1379 - 2195
Palmitic Acid	PCM	58 - 63	55 - 63	8192	8 - 8.71	1692 - 1793
Stearic Acid	PCM	63 - 69	55 - 64	6995	6.26 - 6.77	1560 - 1665
Lithium Bromide	Liquid Absorbent	40	100	2065	3.18	4483
Lithium Chloride	Liquid Absorbent	100	97	1616	0.99	1743
Potassium Hydroxide	Liquid Absorbent	95	100	2065	1.33	1881
Sodium Hydroxide	Liquid Absorbent	95	100	3200	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	54	1662	1.02	973
Magnesium Chloride	Chemical Adsorbent	100	53	1163	0.71	954
Magnesium Sulfate	Chemical Adsorbent	100	53	760	0.47	954
Silica Gel	Solid Physical Adsorbent	100	86	12929	7.94	1541
Zeolite 13X	Solid Physical Adsorbent	96	100	4254	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	75	8401	5.16	1350
Zeolite 4A	Solid Physical Adsorbent	87	100	6068	4.29	2060

Table S20: Horsetail well results from waste heat storage modelling

WH (GJ):	2569.61	MD Modules:	41
FPW_{day} (m^3/day):	74.6	Minimum GOR:	3.15
		Critical SEC (kJ/kg):	718

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	19 - 25	37 - 62	9079	7.98 - 10.47	1369 - 1742
Paraffin Wax	PCM	11 - 26	21 - 74	13596	11.47 - 27.21	1369 - 2013
n-Pentacosane	PCM	8 - 25	15 - 78	8114	7.32 - 22.88	1372 - 2247
n-Hexacozane	PCM	8 - 26	15 - 78	7635	6.55 - 22.31	1367 - 2136
n-Heptacozane	PCM	8 - 27	15 - 77	8520	7 - 25.02	1371 - 2031
n-Nonacozane	PCM	28 - 30	67 - 77	7842	5.82 - 6.35	1747 - 1845
n-Triacontane	PCM	29 - 31	68 - 78	8078	5.74 - 6.2	1682 - 1775
Myristic Acid	PCM	9 - 25	17 - 75	8557	7.74 - 21.99	1378 - 2192
Palmitic Acid	PCM	28 - 31	67 - 77	9040	6.56 - 7.14	1692 - 1792
Stearic Acid	PCM	31 - 33	67 - 77	7719	5.19 - 5.62	1560 - 1664
Lithium Bromide	Liquid Absorbent	16	100	2279	3.18	4483
Lithium Chloride	Liquid Absorbent	41	100	1783	0.97	1743
Potassium Hydroxide	Liquid Absorbent	38	100	2279	1.33	1881
Sodium Hydroxide	Liquid Absorbent	38	100	3531	2.07	1881
Calcium Sulfate	Chemical Adsorbent	74	100	1834	0.56	973
Magnesium Chloride	Chemical Adsorbent	75	100	1283	0.38	954
Magnesium Sulfate	Chemical Adsorbent	75	100	838	0.25	954
Silica Gel	Solid Physical Adsorbent	47	100	14266	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	39	100	4695	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	53	100	9270	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	35	100	6696	4.29	2060

Table S21: J Klein well results from waste heat storage modelling

WH (GJ):	2741.38	MD Modules:	20
FPW_{day} (m^3/day):	35.2	Minimum GOR:	1.39
		Critical SEC (kJ/kg):	1622

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	38 - 50	32 - 54	9685	9.21 - 12.1	1369 - 1745
Paraffin Wax	PCM	21 - 51	18 - 63	14505	13.57 - 32.27	1370 - 2015
n-Pentacosane	PCM	16 - 49	13 - 68	8656	8.38 - 26.27	1373 - 2249
n-Hexacozane	PCM	15 - 52	13 - 68	8145	7.47 - 25.53	1368 - 2137
n-Heptacozane	PCM	15 - 54	13 - 67	9090	8.04 - 28.81	1371 - 2032
n-Nonacozane	PCM	55 - 59	59 - 68	8366	6.66 - 7.27	1747 - 1846
n-Triacontane	PCM	57 - 62	60 - 68	8618	6.58 - 7.11	1682 - 1776
Myristic Acid	PCM	17 - 49	14 - 66	9129	8.89 - 25.34	1379 - 2194
Palmitic Acid	PCM	55 - 60	58 - 67	9644	7.57 - 8.24	1692 - 1793
Stearic Acid	PCM	61 - 66	58 - 67	8235	5.94 - 6.43	1560 - 1664
Lithium Bromide	Liquid Absorbent	36	100	2431	3.18	4483
Lithium Chloride	Liquid Absorbent	93	100	1903	0.97	1743
Potassium Hydroxide	Liquid Absorbent	86	100	2431	1.33	1881
Sodium Hydroxide	Liquid Absorbent	86	100	3767	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	60	1957	0.93	973
Magnesium Chloride	Chemical Adsorbent	100	59	1369	0.65	954
Magnesium Sulfate	Chemical Adsorbent	100	59	894	0.42	954
Silica Gel	Solid Physical Adsorbent	100	95	15220	7.20	1541
Zeolite 13X	Solid Physical Adsorbent	87	100	5008	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	83	9890	4.68	1350
Zeolite 4A	Solid Physical Adsorbent	79	100	7144	4.29	2060

Table S22: JZM well results from waste heat storage modelling

WH (GJ):	3994.56	MD Modules:	71
FPW_{day} (m^3/day):	130.7	Minimum GOR:	3.55
		Critical SEC (kJ/kg):	637

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	18 - 23	38 - 64	14113	7.68 - 10.07	1369 - 1742
Paraffin Wax	PCM	10 - 25	22 - 78	21136	10.96 - 25.98	1369 - 2012
n-Pentacosane	PCM	7 - 23	16 - 80	12614	7.06 - 22.05	1372 - 2247
n-Hexacozane	PCM	7 - 24	15 - 80	11869	6.32 - 21.53	1367 - 2136
n-Heptacozane	PCM	7 - 25	15 - 80	13245	6.74 - 24.1	1371 - 2031
n-Nonacozane	PCM	25 - 28	70 - 80	12190	5.62 - 6.12	1746 - 1845
n-Triacontane	PCM	27 - 29	71 - 81	12557	5.53 - 5.97	1682 - 1775
Myristic Acid	PCM	8 - 23	17 - 78	13302	7.46 - 21.19	1378 - 2192
Palmitic Acid	PCM	26 - 28	69 - 80	14053	6.31 - 6.87	1692 - 1792
Stearic Acid	PCM	28 - 31	69 - 80	12000	5.01 - 5.42	1560 - 1663
Lithium Bromide	Liquid Absorbent	14	100	3543	3.18	4483
Lithium Chloride	Liquid Absorbent	37	100	2772	0.97	1743
Potassium Hydroxide	Liquid Absorbent	34	100	3543	1.33	1881
Sodium Hydroxide	Liquid Absorbent	34	100	5490	2.07	1881
Calcium Sulfate	Chemical Adsorbent	65	100	2851	0.56	973
Magnesium Chloride	Chemical Adsorbent	67	100	1994	0.38	954
Magnesium Sulfate	Chemical Adsorbent	67	100	1303	0.25	954
Silica Gel	Solid Physical Adsorbent	41	100	22178	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	34	100	7298	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	47	100	14411	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	31	100	10409	4.29	2060

Table S23: Markham well results from waste heat storage modelling

WH (GJ):	1585.86	MD Modules:	67
FPW_{day} (m^3/day):	123	Minimum GOR:	8.41
		Critical SEC (kJ/kg):	269

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	8 - 10	40 - 66	5603	7.41 - 9.71	1369 - 1741
Paraffin Wax	PCM	5 - 11	23 - 81	8391	10.49 - 24.84	1369 - 2012
n-Pentacosane	PCM	3 - 10	16 - 83	5008	6.82 - 21.27	1372 - 2246
n-Hexacozane	PCM	3 - 10	16 - 83	4712	6.11 - 20.79	1366 - 2135
n-Heptacozane	PCM	3 - 11	16 - 83	5258	6.51 - 23.23	1370 - 2030
n-Nonacozane	PCM	11 - 12	72 - 83	4840	5.43 - 5.92	1746 - 1844
n-Triacontane	PCM	12 - 13	73 - 84	4985	5.34 - 5.77	1682 - 1774
Myristic Acid	PCM	4 - 10	18 - 81	5281	7.2 - 20.42	1378 - 2191
Palmitic Acid	PCM	11 - 12	72 - 83	5579	6.09 - 6.62	1691 - 1791
Stearic Acid	PCM	12 - 13	72 - 83	4764	4.84 - 5.24	1559 - 1663
Lithium Bromide	Liquid Absorbent	6	100	1406	3.18	4483
Lithium Chloride	Liquid Absorbent	15	100	1101	0.97	1743
Potassium Hydroxide	Liquid Absorbent	14	100	1406	1.33	1881
Sodium Hydroxide	Liquid Absorbent	14	100	2179	2.07	1881
Calcium Sulfate	Chemical Adsorbent	28	100	1132	0.56	973
Magnesium Chloride	Chemical Adsorbent	28	100	792	0.38	954
Magnesium Sulfate	Chemical Adsorbent	28	100	517	0.25	954
Silica Gel	Solid Physical Adsorbent	17	100	8804	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	14	100	2897	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	20	100	5721	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	13	100	4133	4.29	2060

Table S24: Orr State well results from waste heat storage modelling

WH (GJ):	2416.89	MD Modules:	9
FPW_{day} (m^3/day):	15.1	Minimum GOR:	0.68
		Critical SEC (kJ/kg):	3343

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	61 - 81	25 - 42	8539	11.73 - 15.44	1370 - 1747
Paraffin Wax	PCM	33 - 79	14 - 48	12788	17.86 - 42.62	1370 - 2017
n-Pentacosane	PCM	25 - 80	10 - 54	7632	10.54 - 33.2	1373 - 2251
n-Hexacozane	PCM	25 - 85	10 - 54	7181	9.36 - 32.11	1368 - 2139
n-Heptacozane	PCM	24 - 87	10 - 53	8014	10.17 - 36.57	1371 - 2034
n-Nonacozane	PCM	89 - 97	47 - 54	7375	8.38 - 9.14	1747 - 1847
n-Triacontane	PCM	94 - 100	47 - 52	7598	8.41 - 8.97	1683 - 1746
Myristic Acid	PCM	28 - 79	11 - 52	8048	11.24 - 32.16	1379 - 2196
Palmitic Acid	PCM	90 - 98	45 - 52	8503	9.63 - 10.5	1692 - 1794
Stearic Acid	PCM	99 - 100	46 - 47	7260	8.03 - 8.09	1560 - 1564
Lithium Bromide	Liquid Absorbent	75	100	2144	3.18	4483
Lithium Chloride	Liquid Absorbent	100	52	1677	1.86	1743
Potassium Hydroxide	Liquid Absorbent	100	56	2144	2.37	1881
Sodium Hydroxide	Liquid Absorbent	100	56	3321	3.67	1881
Calcium Sulfate	Chemical Adsorbent	100	29	1725	1.91	973
Magnesium Chloride	Chemical Adsorbent	100	29	1207	1.34	954
Magnesium Sulfate	Chemical Adsorbent	100	29	789	0.87	954
Silica Gel	Solid Physical Adsorbent	100	46	13419	14.85	1541
Zeolite 13X	Solid Physical Adsorbent	100	56	4416	4.89	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	40	8720	9.65	1350
Zeolite 4A	Solid Physical Adsorbent	100	62	6298	6.97	2060

Table S25: Puma Fed well results from waste heat storage modelling

WH (GJ):	2589.44	MD Modules:	15
FPW_{day} (m^3/day):	26.1	Minimum GOR:	1.09
		Critical SEC (kJ/kg):	2065

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	45 - 59	30 - 50	9149	9.9 - 13.01	1370 - 1745
Paraffin Wax	PCM	25 - 59	17 - 58	13701	14.74 - 35.09	1370 - 2015
n-Pentacosane	PCM	19 - 58	12 - 63	8177	8.97 - 28.16	1373 - 2250
n-Hexacozane	PCM	18 - 61	12 - 64	7694	7.99 - 27.32	1368 - 2138
n-Heptacozane	PCM	18 - 64	12 - 63	8586	8.62 - 30.93	1371 - 2033
n-Nonacozane	PCM	65 - 71	55 - 63	7902	7.13 - 7.78	1747 - 1846
n-Triacontane	PCM	68 - 74	56 - 63	8140	7.04 - 7.61	1682 - 1776
Myristic Acid	PCM	20 - 58	14 - 61	8623	9.53 - 27.2	1379 - 2195
Palmitic Acid	PCM	66 - 71	54 - 62	9110	8.13 - 8.86	1692 - 1793
Stearic Acid	PCM	72 - 78	54 - 63	7779	6.36 - 6.88	1560 - 1665
Lithium Bromide	Liquid Absorbent	46	100	2297	3.18	4483
Lithium Chloride	Liquid Absorbent	100	84	1797	1.15	1743
Potassium Hydroxide	Liquid Absorbent	100	91	2297	1.47	1881
Sodium Hydroxide	Liquid Absorbent	100	91	3559	2.27	1881
Calcium Sulfate	Chemical Adsorbent	100	47	1848	1.18	973
Magnesium Chloride	Chemical Adsorbent	100	46	1293	0.82	954
Magnesium Sulfate	Chemical Adsorbent	100	46	845	0.54	954
Silica Gel	Solid Physical Adsorbent	100	75	14377	9.17	1541
Zeolite 13X	Solid Physical Adsorbent	100	90	4731	3.02	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	65	9342	5.96	1350
Zeolite 4A	Solid Physical Adsorbent	100	100	6748	4.30	2060

Table S26: RBF well results from waste heat storage modelling

WH (GJ):	2179.49	MD Modules:	15
FPW_{day} (m^3/day):	26.8	Minimum GOR:	1.33
		Critical SEC (kJ/kg):	1697

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	38 - 50	31 - 51	7700	9.64 - 12.67	1370 - 1745
Paraffin Wax	PCM	21 - 50	17 - 60	11532	14.3 - 34.03	1370 - 2015
n-Pentacosane	PCM	16 - 49	13 - 65	6882	8.75 - 27.45	1373 - 2249
n-Hexacozane	PCM	15 - 52	12 - 65	6476	7.79 - 26.65	1368 - 2137
n-Heptacozane	PCM	15 - 54	12 - 64	7227	8.4 - 30.13	1371 - 2032
n-Nonacozane	PCM	55 - 60	56 - 65	6651	6.95 - 7.59	1747 - 1846
n-Triacontane	PCM	58 - 62	57 - 65	6852	6.87 - 7.42	1682 - 1776
Myristic Acid	PCM	17 - 49	14 - 63	7258	9.29 - 26.49	1379 - 2194
Palmitic Acid	PCM	55 - 60	55 - 64	7668	7.92 - 8.63	1692 - 1793
Stearic Acid	PCM	61 - 66	56 - 65	6547	6.2 - 6.71	1560 - 1664
Lithium Bromide	Liquid Absorbent	38	100	1933	3.18	4483
Lithium Chloride	Liquid Absorbent	97	100	1513	0.97	1743
Potassium Hydroxide	Liquid Absorbent	90	100	1933	1.33	1881
Sodium Hydroxide	Liquid Absorbent	90	100	2995	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	57	1556	0.97	973
Magnesium Chloride	Chemical Adsorbent	100	56	1088	0.68	954
Magnesium Sulfate	Chemical Adsorbent	100	56	711	0.44	954
Silica Gel	Solid Physical Adsorbent	100	91	12100	7.54	1541
Zeolite 13X	Solid Physical Adsorbent	91	100	3982	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	80	7863	4.90	1350
Zeolite 4A	Solid Physical Adsorbent	82	100	5680	4.29	2060

Table S27: Stromberger well results from waste heat storage modelling

WH (GJ):	5828.74	MD Modules:	7
FPW_{day} (m^3/day):	12.9	Minimum GOR:	0.24
		Critical SEC (kJ/kg):	9437

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	100	13	20593	26.67	1259
Paraffin Wax	PCM	63 - 100	9 - 18	30841	39.95 - 63.1	1370 - 1742
n-Pentacosane	PCM	51 - 100	7 - 21	18406	23.84 - 46.92	1373 - 1966
n-Hexacozane	PCM	50 - 100	7 - 20	17319	22.43 - 45.12	1368 - 1873
n-Heptacozane	PCM	48 - 100	7 - 19	19326	25.03 - 51.91	1372 - 1798
n-Nonacozane	PCM	100	17	17788	23.04	1616
n-Triacontane	PCM	100	17	18323	23.73	1572
Myristic Acid	PCM	55 - 100	8 - 20	19410	25.14 - 45.67	1379 - 1898
Palmitic Acid	PCM	100	16	20506	26.56	1545
Stearic Acid	PCM	100	16	17510	22.68	1468
Lithium Bromide	Liquid Absorbent	100	48	5169	6.70	4483
Lithium Chloride	Liquid Absorbent	100	18	4045	5.24	1743
Potassium Hydroxide	Liquid Absorbent	100	20	5169	6.70	1881
Sodium Hydroxide	Liquid Absorbent	100	20	8010	10.38	1881
Calcium Sulfate	Chemical Adsorbent	100	10	4161	5.39	973
Magnesium Chloride	Chemical Adsorbent	100	10	2910	3.77	954
Magnesium Sulfate	Chemical Adsorbent	100	10	1902	2.46	954
Silica Gel	Solid Physical Adsorbent	100	16	32361	41.92	1541
Zeolite 13X	Solid Physical Adsorbent	100	20	10649	13.79	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	14	21029	27.24	1350
Zeolite 4A	Solid Physical Adsorbent	100	22	15189	19.67	2060

Table S28: TC Hiland Knolls well results from waste heat storage modelling

WH (GJ):	3750.09	MD Modules:	33
FPW_{day} (m^3/day):	60.5	Minimum GOR:	1.75
		Critical SEC (kJ/kg):	1292

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	33 - 43	35 - 58	13249	8.54 - 11.22	1369 - 1743
Paraffin Wax	PCM	19 - 44	20 - 69	19842	12.43 - 29.52	1370 - 2014
n-Pentacosane	PCM	13 - 42	14 - 73	11842	7.8 - 24.43	1373 - 2248
n-Hexacozane	PCM	13 - 44	14 - 73	11143	6.97 - 23.79	1367 - 2137
n-Heptacozane	PCM	13 - 46	14 - 72	12434	7.47 - 26.75	1371 - 2032
n-Nonacozane	PCM	47 - 51	63 - 73	11444	6.21 - 6.77	1747 - 1845
n-Triacontane	PCM	49 - 53	64 - 73	11789	6.12 - 6.61	1682 - 1775
Myristic Acid	PCM	15 - 42	16 - 71	12488	8.27 - 23.52	1379 - 2193
Palmitic Acid	PCM	48 - 52	62 - 72	13193	7.02 - 7.64	1692 - 1792
Stearic Acid	PCM	52 - 56	63 - 72	11265	5.53 - 5.99	1560 - 1664
Lithium Bromide	Liquid Absorbent	29	100	3326	3.18	4483
Lithium Chloride	Liquid Absorbent	74	100	2603	0.97	1743
Potassium Hydroxide	Liquid Absorbent	69	100	3326	1.33	1881
Sodium Hydroxide	Liquid Absorbent	69	100	5153	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	75	2677	0.74	973
Magnesium Chloride	Chemical Adsorbent	100	74	1872	0.52	954
Magnesium Sulfate	Chemical Adsorbent	100	74	1223	0.34	954
Silica Gel	Solid Physical Adsorbent	84	100	20820	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	69	100	6851	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	96	100	13529	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	63	100	9772	4.29	2060

Table S29: Wells Ranch well results from waste heat storage modelling

WH (GJ):	7866.87	MD Modules:	36
FPW_{day} (m^3/day):	65.7	Minimum GOR:	0.91
		Critical SEC (kJ/kg):	2494

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	59 - 77	32 - 54	27794	9.12 - 11.98	1369 - 1744
Paraffin Wax	PCM	33 - 79	18 - 64	41624	13.41 - 31.88	1370 - 2014
n-Pentacosane	PCM	24 - 76	13 - 68	24842	8.3 - 26.01	1373 - 2249
n-Hexacozane	PCM	23 - 80	13 - 69	23375	7.4 - 25.28	1368 - 2137
n-Heptacozane	PCM	23 - 83	13 - 68	26085	7.96 - 28.53	1371 - 2032
n-Nonacozane	PCM	85 - 92	59 - 68	24007	6.6 - 7.2	1747 - 1846
n-Triacontane	PCM	89 - 96	60 - 69	24730	6.51 - 7.04	1682 - 1776
Myristic Acid	PCM	26 - 75	15 - 66	26197	8.8 - 25.08	1379 - 2194
Palmitic Acid	PCM	86 - 94	58 - 67	27676	7.49 - 8.16	1692 - 1793
Stearic Acid	PCM	94 - 100	59 - 65	23633	5.99 - 6.36	1560 - 1622
Lithium Bromide	Liquid Absorbent	56	100	6977	3.18	4483
Lithium Chloride	Liquid Absorbent	100	70	5460	1.38	1743
Potassium Hydroxide	Liquid Absorbent	100	75	6977	1.77	1881
Sodium Hydroxide	Liquid Absorbent	100	75	10811	2.74	1881
Calcium Sulfate	Chemical Adsorbent	100	39	5616	1.42	973
Magnesium Chloride	Chemical Adsorbent	100	38	3928	1.00	954
Magnesium Sulfate	Chemical Adsorbent	100	38	2567	0.65	954
Silica Gel	Solid Physical Adsorbent	100	62	43676	11.08	1541
Zeolite 13X	Solid Physical Adsorbent	100	75	14372	3.65	1863
Zeolite 13XBF	Solid Physical Adsorbent	100	54	28382	7.20	1350
Zeolite 4A	Solid Physical Adsorbent	100	83	20500	5.20	2060

Table S30: Wilson Ranch well results from waste heat storage modelling

WH (GJ):	2488.18	MD Modules:	24
FPW_{day} (m^3/day):	42.8	Minimum GOR:	1.87
		Critical SEC (kJ/kg):	1210

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	30 - 39	34 - 56	8791	8.73 - 11.46	1369 - 1744
Paraffin Wax	PCM	17 - 40	19 - 67	13165	12.75 - 30.28	1370 - 2014
n-Pentacosane	PCM	12 - 38	14 - 71	7857	7.96 - 24.94	1373 - 2248
n-Hexacozane	PCM	12 - 40	13 - 71	7393	7.11 - 24.26	1368 - 2137
n-Heptacozane	PCM	12 - 42	13 - 71	8250	7.63 - 27.33	1371 - 2032
n-Nonacozane	PCM	43 - 47	62 - 71	7593	6.33 - 6.91	1747 - 1845
n-Triacontane	PCM	45 - 49	63 - 71	7822	6.25 - 6.75	1682 - 1775
Myristic Acid	PCM	13 - 38	15 - 69	8286	8.44 - 24.02	1379 - 2193
Palmitic Acid	PCM	44 - 47	61 - 70	8754	7.17 - 7.81	1692 - 1793
Stearic Acid	PCM	48 - 51	61 - 71	7475	5.65 - 6.11	1560 - 1664
Lithium Bromide	Liquid Absorbent	27	100	2207	3.18	4483
Lithium Chloride	Liquid Absorbent	69	100	1727	0.97	1743
Potassium Hydroxide	Liquid Absorbent	64	100	2207	1.33	1881
Sodium Hydroxide	Liquid Absorbent	64	100	3419	2.07	1881
Calcium Sulfate	Chemical Adsorbent	100	80	1776	0.69	973
Magnesium Chloride	Chemical Adsorbent	100	79	1242	0.48	954
Magnesium Sulfate	Chemical Adsorbent	100	79	812	0.32	954
Silica Gel	Solid Physical Adsorbent	79	100	13814	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	65	100	4546	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	90	100	8977	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	59	100	6484	4.29	2060

Table S31: Woolley Sosa well results from waste heat storage modelling

WH (GJ):	2669.17	MD Modules:	41
FPW_{day} (m^3/day):	57.6	Minimum GOR:	2.03
		Critical SEC (kJ/kg):	1111

Storage Material	Type	FPW_{treat}	WH_{util}	V_{store}	Inverse Volumetric Treatment Capacity	$ASEC$
-	-	%	%	m^3	m^3/m^3	kJ/kg
Water	SSM	25 - 33	35 - 59	9430	8.32 - 10.92	1369 - 1743
Paraffin Wax	PCM	14 - 34	20 - 71	14123	12.05 - 28.6	1370 - 2013
n-Pentacosane	PCM	10 - 32	15 - 75	8429	7.61 - 23.81	1373 - 2248
n-Hexacozane	PCM	10 - 34	14 - 75	7931	6.8 - 23.2	1367 - 2136
n-Heptacozane	PCM	10 - 35	14 - 74	8850	7.28 - 26.06	1371 - 2032
n-Nonacozane	PCM	36 - 39	65 - 74	8145	6.05 - 6.6	1747 - 1845
n-Triacontane	PCM	38 - 41	66 - 75	8391	5.97 - 6.45	1682 - 1775
Myristic Acid	PCM	11 - 32	16 - 73	8888	8.06 - 22.91	1379 - 2193
Palmitic Acid	PCM	37 - 40	64 - 74	9390	6.84 - 7.44	1692 - 1792
Stearic Acid	PCM	40 - 43	64 - 74	8018	5.4 - 5.84	1560 - 1664
Lithium Bromide	Liquid Absorbent	22	100	2367	3.18	4483
Lithium Chloride	Liquid Absorbent	55	100	1852	0.97	1743
Potassium Hydroxide	Liquid Absorbent	51	100	2367	1.33	1881
Sodium Hydroxide	Liquid Absorbent	51	100	3668	2.07	1881
Calcium Sulfate	Chemical Adsorbent	99	100	1905	0.56	973
Magnesium Chloride	Chemical Adsorbent	100	99	1333	0.39	954
Magnesium Sulfate	Chemical Adsorbent	100	99	871	0.25	954
Silica Gel	Solid Physical Adsorbent	63	100	14819	6.84	1541
Zeolite 13X	Solid Physical Adsorbent	52	100	4876	2.72	1863
Zeolite 13XBF	Solid Physical Adsorbent	71	100	9630	3.90	1350
Zeolite 4A	Solid Physical Adsorbent	47	100	6955	4.29	2060

S.4. Economic and Environmental Evaluations

S.4.1. Technology Models

S.4.1.1. Mechanical Vapor Compression Model

Table S32: MVC Model Inputs for Average Scenario Na_2SO_4 Removal

Input	Value	Unit
Salt Type	Na_2SO_4	-
Inlet Flowrate	10.42	kg/s
Inlet Salinity	68,500	ppm
Compressor efficiencies	0.70	-
Brine Salinity	100,000	ppm

ASPEN Plus allows for additional restrictions on model operation to be defined. These restrictions are called Design Specifications within the program. When the simulations are solved, the program will follow the thermodynamic and chemical operations of every piece of equipment in the system, and then iterate solutions to account for the additional design specifications. The design specifications used are outlined in Table S33.

Table S33: MVC Model Design Restrictions/Design Specifications

Design Specification	Manipulated Variable	Explanation
$T_{16} - T_8 = 10$	Compressor compression ratio	This relationship restricts the compression ratio in the compressor block such that the exiting flow has sufficient saturation temperature to allow heat transfer in the evaporator.
$T_4 - T_5 = 0$	Degrees of subcooling at the exits of the first preheater	This limits the amount of heat transfer being done by the first preheater, such that the flows merging into flow 6 have the same temperature.
$Vapfrac_{16} = 0.01$	Degrees of subcooling at the exit of the second preheater	This specification restricts the amount of heating in the evaporator, such that sufficient heat is transferred from flow 15, allowing flow 16 to be almost completely condensed.
$\dot{m}_{Na_2SO_4,1} = \dot{m}_{Na_2SO_4,13}$	$\dot{m}_{11}/\dot{m}_9$	To ensure that there is not an accumulation of salts in the system, all incoming salt mass must leave through the brine at equal rates. The split fractions of flow 9 ensure this balance.
$T_{13} - T_{18} = 0$	$\dot{m}_2/\dot{m}_1$	By changing the fraction of incoming mass flowing through each preheater, it can be ensured that the exit temperature of the clean water stream and the brine stream are equal.
$\dot{m}_{H_2O,1} = \dot{m}_{H_2O,13} + \dot{m}_{H_2O,14}$	$Vapfrac\_evap$	To ensure that there is not an accumulation of water in the system, all incoming water mass must leave through the vapor stream or brine stream at equal rates. This balance is determined by the vapor fraction in the evaporator.

T: temperature
$\dot{m}$: mass flowrate
$Vapfrac$: vapor fraction

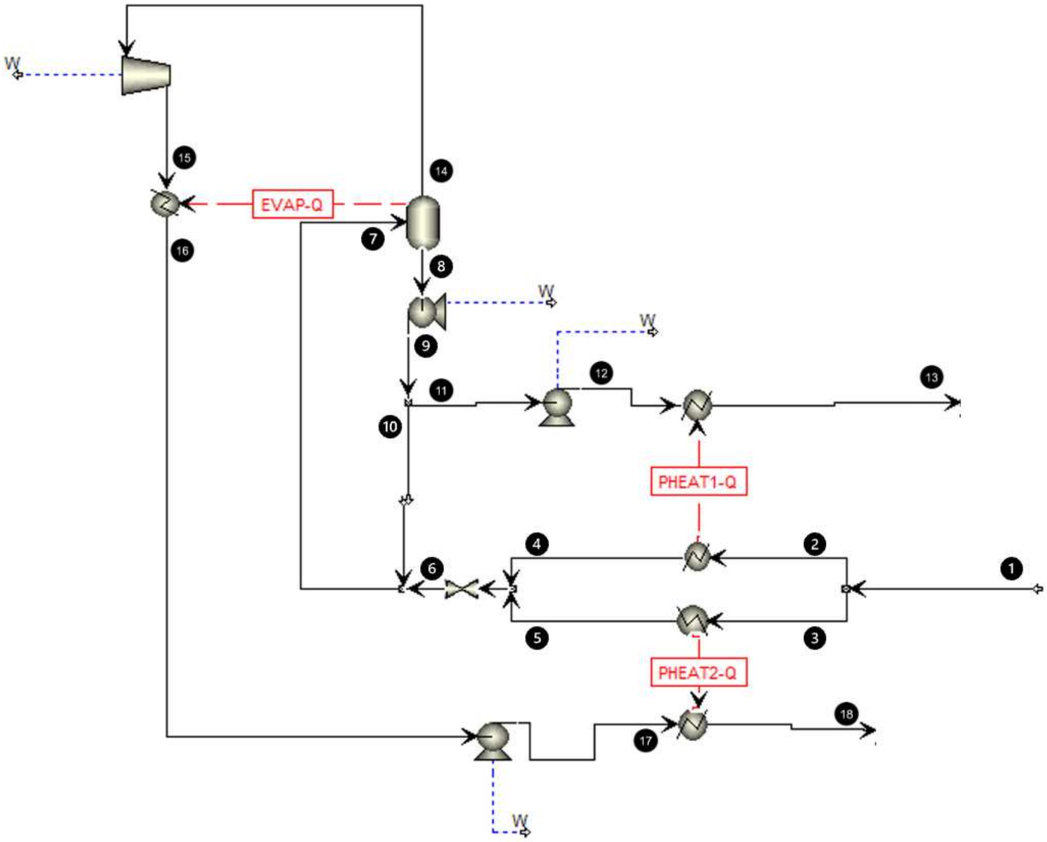

Figure S3: MVC Process Flow Diagram, as organized in ASPEN Plus

Table S34: MVC State Points During Average Scenario Na_2SO_4 Removal

State Point	Temperature	Pressure	Mass Flow	Concentration	Phase (Vapor Fraction)
-	C	kPa	kg/s	ppm	- (-)
1	25.0	101	10.4	68500	Liquid
2	25.0	101	5.8	68500	Liquid
3	25.0	101	4.7	68500	Liquid
4	55.6	101	5.8	68500	Liquid
5	56.2	101	4.7	68500	Liquid
6	55.9	19	10.4	68500	Liquid
7	57.8	19	20.4	83929	Liquid
8	59.9	19	17.1	100000	Liquid
9	59.8	19	17.1	100000	Liquid
10	59.8	19	10.0	100000	Liquid
11	59.8	19	7.1	100000	Liquid
12	59.9	101	7.1	100000	Liquid
13	34.4	101	7.1	100000	Liquid
14	59.9	19	3.3	0	Vapor
15	118.0	30	3.3	0	Vapor
16	69.8	30	3.3	0	Liquid
17	75.3	101	3.3	0	Liquid
18	34.4	101	3.3	0	Liquid

Heat Exchange Rate	kW
PHEAT1-Q	-681.2
PHEAT2-Q	-562.0
EVAP-Q	-7909.1

Note: The negative heat exchange values denote that heat transfer is happening in the opposite direction of the arrow in Figure S3.

Energy Consumption Rate	kW
Compressor	360.0
$Pump_{8-9}$	0.0 (assumed zeros losses)
$Pump_{11-12}$	1.0
$Pump_{16-17}$	12.3

S.4.1.2. Crystallizer Model

Table S35: Crystallizer Model Inputs for Average Scenario Na_2SO_4 Removal after MVC

Input	Value	Unit
Salt Type	Na_2SO_4	-
Inlet Flowrate	7.1	kg/s
Inlet Salinity	100,000	ppm
Compressor efficiencies	0.7	-
Crystallizer Recirculation Rate	100	-

Table S36: Crystallizer Model Design Restrictions/Design Specifications

Design Specification	Manipulated Variable	Explanation
$T_7 - T_4 = 1$	compressor compression ratio	This relationship restricts the compression ratio in the compressor block such that the exiting flow has sufficient saturation temperature to allow heat transfer in the evaporator.
$Vapfrac_7 = 0.01$	Degrees of subcooling in the heater	This specification restricts the amount of heating in the heater, such that sufficient heat is transferred from flow 6, allowing flow 7 to be almost completely condensed.
$EVAPQ = 0$	P_4	In the crystallizer, no heat is added to the evaporator. Rather, evaporation is induced by a sudden decrease in pressure within the evaporator. As such, the pressure of the incoming stream is very important. By changing the incoming pressure, we can ensure sufficient vaporization rates while maintaining zero heat addition in the evaporator.
$\dot{m}_{Na_2SO_4,1} = \dot{m}_{Na_2SO_4,14}$	$\dot{m}$_12/$\dot{m}$_11	To ensure that there is not an accumulation of salts in the system, all incoming salt mass must leave through the brine at equal rates. The split fractions of flow 11 ensure this balance.
$\dot{m}_{H_2O,1} = \dot{m}_{H_2O,5}$	$Vapfrac\_evap$	To ensure that there is not an accumulation of water in the system, all incoming water mass must leave through the vapor stream or brine stream at equal rates. This balance is determined by the vapor fraction in the evaporator.

T: temperature
$\dot{m}$: mass flowrate
$Vapfrac$: vapor fraction
$EVAPQ$: evaporator heat addition
P: pressure

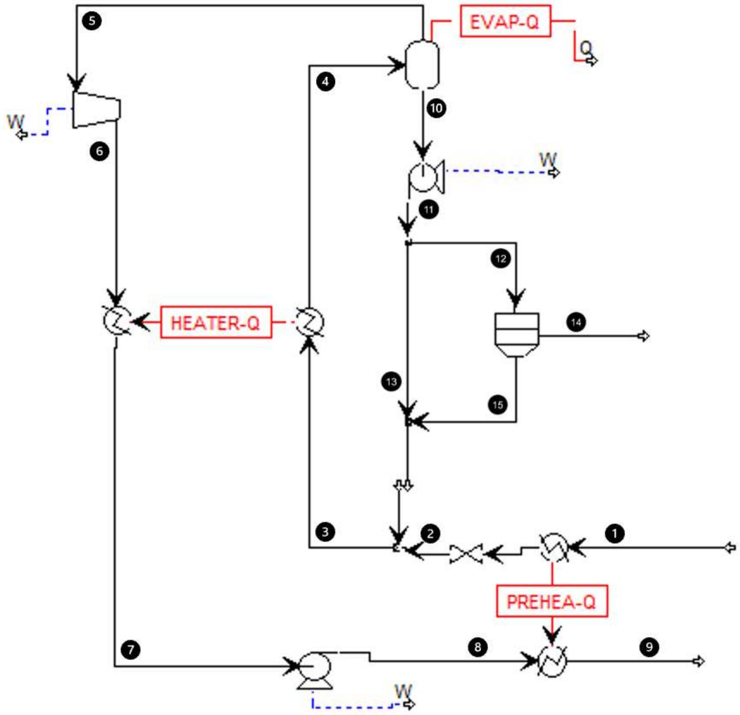

Figure S4: Crystallizer Process Flow Diagram, as organized in ASPEN Plus

Table S37: Crystallizer State Points for Average Scenario Na_2SO_4 Removal

State Point	Temperature	Pressure	Mass Flow	Concentration	Phase (Vapor Fraction)
-	C	kPa	kg/s	ppm	- (-)
1	25.0	23	7.1	100000	Liquid
2	45.2	23	7.1	100000	Liquid
3	57.1	23	720.7	496040	Magma
4	65.2	23	720.7	496040	Magma
5	57.2	15.8	6.4	0	Vapor
6	120.4	26.5	6.4	0	Vapor
7	66.2	26.5	6.4	0	Liquid-Vapor Mixture
8	73.5	101.3	6.4	0	Liquid
9	53.4	101.3	6.4	0	Liquid
10	57.2	15.8	714.3	500500	Magma
11	57.2	23.0	714.3	500500	Magma
12	57.2	23.0	2.4	500500	Magma
13	57.2	23.0	711.9	500500	Magma
14	57.2	23.0	0.7	971326	Magma
15	57.2	23.0	1.6	283152	Liquid

Heat Exchange Rate	kW
PHEAT-Q	-540.1
HEATER-Q	-15571.9
EVAP-Q	0

Note: The negative heat exchange values denote that heat transfer is happening in the opposite direction of the arrow in Figure S4.

Energy Consumption Rate	kW
Compressor	767.1
Pump$_{7-8}$	35.6
Pump$_{10-11}$	4.0

S.4.1.3. Membrane Distillation

The membrane distillation model used in this study was developed by us and previously published in Robbins et al. [5]. The necessary inputs for this model are listed in Table S38. Note that some inputs are not changed in the different scenarios of this study.

Table S38: MD Model Inputs for Average Scenario Na_2SO_4 Removal

Input	Value	Unit	Held constant in this study?
Salt Type	Na_2SO_4	-	No
Inlet Flowrate	10.42	kg/s	No
Inlet Salinity	68,500	ppm	No
Inlet Temperature (T_3)	65	C	No
Recovery Rate	62.5	%	No
Membrane Pore Size	0.45	μm	Yes
Membrane Porosity	75	%	Yes
Membrane Thickness	125	μm	Yes
Membrane Permeability	0.00038	$kg/(m^2 * s * kPa)$	Yes
Membrane Thermal Conductivity	0.09004	$W/(m * K)$	Yes
Heat Exchanger Effectivenesses	0.8	$-$	Yes
Permeate Temperature	20	C	Yes
Heat Exchanger Overall Heat Transfer Coefficients	350	$W/(m^2 * K)$	Yes

S.4.1.4. Electroanalytic Crystallization

The electrodialytic crystallization model used in this study was developed by and previously published by Zhang et al. [57]. The necessary inputs for this model are listed in Table S39. Note that some inputs are not changed in the different scenarios of this study.

Table S39: EDC Model Inputs for Average Scenario Na_2SO_4 Removal

Input	Value	Unit	Held constant in this study?
Salt Type	Na_2SO_4	-	No
Inlet Flowrate	10.42	kg/s	No
Inlet Salinity	68,500	ppm	No
Current Density	200	amp/m^2	No
Crystal Yield	0.6	-	No
Temperature Drop in Crystallization Tank	2	$°C$	No
Water Recovery in the RO Unit	50	%	Yes
Pressure Exchanger Efficiency	85	%	Yes
Finite Pressure Difference at the End of the RO module	5	bar	Yes
Pump Efficiency	60	%	Yes
Membrane Electrical Resistance	3	ohm/cm^2	Yes
Channel Thickness	1	mm	Yes
Brine Stream Concentration	250,000	ppm	Yes
Temperature Drop Efficiency	70	%	Yes

In addition to this model, the size of the crystallization tank was calculated based on the crystallization tank retention time using eq. S1.

$$Size[m^3] = \dot{V}_4[\frac{m^3}{s}] * Retention[h] * \frac{3600[s]}{1[h]} \qquad eq.\ S1$$

S.4.2. Cost Models

The equations used to calculate equipment and variable costs are shared in Table S40. In addition to the equipment costs shared in eq. S2 through eq. S18, an installation factor of 1.3 is used. The total equipment costs are those calculated in Table S40 plus an additional 30% for installation costs. Furthermore, the cost year is updated using the Chemical Engineering Plant Cost Index (CEPCI) as a guide [200]. Table S41 shows the component costs, including both installation costs and normalization of the cost year to 2022. The area of all heat exchangers was determined using a log-mean temperature difference methodology, meaning that area was ultimately determined by total energy transfer within the heat exchanger.

Table S40: Equations Used to Determine Equipment and Variable Costs for All ZLD Technologies

	Component	Cost Equation		Notes and References
		Equipment Costs ($)		
MVC	Centrifugal Compressor	$580{,}000 + 20{,}000 * \dot{W}^{0.6}$	eq. S2	$\dot{W}$ – power supplied to the compressor in kW [201]
	Falling Film Evaporator	$(330 \ + \ 36{,}000 * A^{0.55}) * 1.7$	eq. S3	A – total area of the evaporator in m^2 [202], [201]
	Plate and Frame Heat Exchanger	$(1{,}600 + 210 * A^{0.95})$	eq. S4	A – total area of the heat exchanger in m^2 [201]
Crystallizer	Centrifugal Compressor	$580{,}000 + 20{,}000 * \dot{W}^{0.6}$	eq. S5	$\dot{W}$ – power supplied to the compressor in kW [201]
	Heater	$(28{,}000 + 54 * A^{1.2}) * 1.7$	eq. S6	A – total area of the heater in m^2 [202], [201]
	Plate and Frame Heat Exchanger	$(1{,}600 + 210 * A^{0.95})$	eq. S7	A – total area of the heat exchanger in m^2 [201]
	Separator	$1{,}650 * \frac{\dot{m}}{2.78}$	eq. S8	$\dot{m}$ – mass flowrate through separator in kg/s [203]
	Crystallizer	$1{,}970{,}000 * \left(\frac{\dot{m}}{1.39}\right)^{0.75}$	eq. S9	$\dot{m}$ – dry mass produced in kg/s [203]
ED	Membranes	$C_m * A$	eq. S10	C_m – cost of IEM in $\$/m^2$ A – total area of IEM in m^2 [133]
	Stacks	$1.5 * C_m * A$	eq. S11	C_m – cost of IEM in $\$/m^2$ A – total area of IEM in m^2 [133]
	Axillary Equipment	$0.5 * C_m * A$	eq. S12	C_m – cost of IEM in $\$/m^2$ A – total area of IEM in m^2 [133]
	Crystallization Tank	$6000 * V^{0.71} * rounddn\left(\frac{V}{10{,}000}\right)^{1-0.71}$	eq. S13	V – volume of crystallization tank in gal [202]
RO	Membranes and Permeator	$10 * A$	eq. S14	A – total area of the RO membrane in m^2 [133]
	Pump	$52 * P * \dot{V}$	eq. S15	P – pressure applied in bar $\dot{V}$ – volumetric flow at inlet of RO in m^3/day [133]
MD	Membranes	$83.93 * A$	eq. S16	A – total area of membrane in m^2 [204]
	Membrane Modules	$116.01 * A$	eq. S17	A – total area of membrane in m^2 [204]
	Heat Exchangers	$(1{,}600 + 210 * A^{0.95})$	eq. S18	A – total area of the heat exchanger in m^2 [201]
	Waste Heat Collection and Delivery Technology	$\dot{Q} * (\frac{1{,}634{,}675}{7857})$	eq. S19	$\dot{Q}$ – total waste heat consumption rate of the MD module in kW_{th} [205]
	Component	**Cost Equation**		**Notes and References**
		Variable Costs ($\$/yr$)		
	Electricity	$W * C_E$	eq. S20	W – Energy consumption in kWh/yr C_E – cost of energy in $\$/kWh$
	MVC Pretreatment Chemicals	$0.628 * m$	eq. S21	m – mass of chemicals consumed in kg/yr [206]
	EDC Pretreatment Chemicals	$0.172 * m$	eq. S22	m – mass of chemicals consumed in kg/yr [207],[142]
	RO Cleaning Chemicals	$0.332 * m$	eq. S23	m – mass of chemicals consumed in kg/yr [208]
	Final Disinfection Chemicals	$0.330 * m$	eq. S24	m – mass of chemicals consumed in kg/yr [209]
	Membrane Replacements	$C_m * A * f_{rep}/100$	eq. S25	C_m – cost of membrane in $\$/m^2$ A – area of total membrane in m^2 f_{rep}- replacement factor of membrane in $\%/yr$

Table S41: Average Scenario Component Costs When Removing Na_2SO_4

ZLD Technology	Component	Value	Units
MVC + Crystallizer	**Primary Equipment Costs**		
	Centrifugal Compressor	1,899,376	$\$/lifetime$
	Falling Film Evaporator	1,095,523	$\$/lifetime$
	Plate and Frame Heat Exchanger	8,779	$\$/lifetime$
	Secondary Equipment Costs		
	Centrifugal Compressor	2,489,712	$\$/lifetime$
	Heater	122,898	$\$/lifetime$
	Plate and Frame Heat Exchanger	3,531	$\$/lifetime$
	Separator	181,728	$\$/lifetime$
	Crystallizer	1602,397	$\$/lifetime$
	Primary Variable Costs		
	MVC Electricity	220,747	$\$/year$
	Pretreatment Chemicals	9,329	$\$/year$
	Secondary Variable Costs		
	Crystallizer Electricity	470,401	$\$/year$
	Final Disinfection Chemicals	866	$\$/year$
EDC	**Primary Equipment Costs**		
	Membranes	2,425,400	$\$/lifetime$
	Stacks	3,638,100	$\$/lifetime$
	Axillary Equipment	1,576,510	$\$/lifetime$
	Crystallization Tank	207,242	$\$/lifetime$
	Secondary Equipment Costs		
	Membranes and Permeator	92,430	$\$/lifetime$
	Pump	610,538	$\$/lifetime$
	Primary Variable Costs		
	ED Electricity	235,135	$\$/year$
	Ion Exchange Membrane Replacement	139,927	$\$/year$
	Pretreatment Chemicals	66,470	$\$/year$
	Secondary Variable Costs		
	RO Electricity	50,036	$\$/year$
	RO Membrane Replacement	17,775	$\$/year$
	RO Cleaning Chemicals	54,016	$\$/year$
	Final Disinfection Chemicals	866	$\$/year$
MD + Crystallizer *Waste heat collection and delivery technology cost is only considered in the MD+C w/ WH technology. All other costs shared here are based on the MD+C system when using electrical resistive heating.	**Primary Equipment Costs**		
	Membranes	548,000	$\$/lifetime$
	Membrane Modules	757,458	$\$/lifetime$
	Supply Heat Exchanger	1,562,108	$\$/lifetime$
	Recovery Heat Exchanger	2,632,218	$\$/lifetime$
	Waste Heat Collection and Delivery Technology*	4,480,252	$\$/lifetime$
	Secondary Equipment Costs		
	Centrifugal Compressor	1,742,656	$\$/lifetime$
	Heater	78,198	$\$/lifetime$
	Plate and Frame Heat Exchanger	7,729	$\$/lifetime$
	Separator	89,624	$\$/lifetime$
	Crystallizer	942,451	$\$/lifetime$
	Primary Variable Costs		
	MD Electricity	9,309,781	$\$/year$
	MD Membrane Replacement	42,154	$\$/year$
	Secondary Variable Costs		
	Crystallizer Electricity	167,538	$\$/year$
	Final Disinfection Chemicals	866	$\$/year$

Table S42: Values Used for All DCFROR Analysis in This Study [139]

Variable	Value	Units
Equity	40	%
Loan term	10	years
Loan interest	8	%
Tax depreciation framework	MARCS 7 year	-
Construction period	3	years
Startup time	0.5	years
Startup rate	40	%
Internal rate of return	10	%
Tax rate	35	%

S.4.3. Life Cycle Inventory and Impacts

Table S43: Life Cycle Inventory for Technologies when Removing Na_2SO_4 in the Average Operating Scenario

ZLD Technology	Component	Value	Units
MVC + Crystallizer	Electricity	30.056	kWh/m^3
	MVC Pretreatment Chemicals	0.047	kg/m^3
	Final Disinfection Chemicals	0.008	kg/m^3
EDC	Electricity	12.401	kWh/m^3
	ED Pretreatment Chemicals	0.970	kg/m^3
	RO Cleaning Chemicals	0.196	kg/m^3
	Final Disinfection Chemicals	0.008	kg/m^3
	Ion Exchange Membrane Replacement	0.004	m^2/m^3
	RO Membrane Replacement	0.005	m^2/m^3
MD + Crystallizer	Electricity	412.147	kWh/m^3
	Final Disinfection Chemicals	0.008	kg/m^3
	MD Membrane Replacement	0.002	m^2/m^3

Table S44: Life Cycle Impacts: GWP of Life Cycle Components from Inventory [141]

Component	Value	Units
Electricity	0.47	kg CO_2 eq/kWh
MVC Pretreatment Chemicals	1.27	kg CO_2 eq /kg
Final Disinfection Chemicals	2.49	kg CO_2 eq /kg
ED Pretreatment Chemicals	1.24	kg CO_2 eq /kg
RO Cleaning Chemicals	0.89	kg CO_2 eq /kg
Ion Exchange Membrane Replacement	27.78	kg CO_2 eq /m^2
RO Membrane Replacement	87.49	kg CO_2 eq /m^2
MD Membrane Replacement	0.28	kg CO_2 eq /m^2

S.4.4. Additional Results

S.4.4.1. Na_2SO_4 Crystallization

S.4.4.1.1. TEA

Table S45: Levelized cost of water in a Na_2SO_4 removal process [$/m^3]

ZLD Technology	**Average Cost**	**Conservative Cost**	**Optimistic Cost**
Total Cost (Sum of Capital and Operational Costs)			
MVC + Crystallizer	10.79	13.45	9.12
EDC	12.11	66.59	3.55
MD + Crystallizer	40.32	136.44	20.07
MD + Crystallizer w/ WH	16.17	54.93	9.31
Capital Cost (Equipment/All Other)			
MVC + Crystallizer	3.87/3.41	4.55/4.00	3.40/3.00
EDC	4.68/4.12	29.09/25.60	1.08/0.95
MD + Crystallizer	4.51/3.44	15.52/13.66	2.56/1.95
MD + Crystallizer w/ WH	7.14/6.28	25.72/22.63	3.89/3.43
Operational Cost (Energy/All Other)			
MVC + Crystallizer	2.38/1.14	3.56/1.33	1.72/1.00
EDC	1.01/2.30	1.31/10.59	0.64/0.88
MD + Crystallizer	31.04/1.32	103.20/4.06	14.76/0.81
MD + Crystallizer w/ WH	0.60/2.19	0.18/6.40	0.70/1.28

Table S46: Sensitivity of LCOW in Na_2SO_4 removal process using MVC+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.8%	-0.8%	0.6%	-0.6%	0.4%	-0.4%
Inlet Salinity	0.3%	-0.5%	-0.3%	0.0%	-1.4%	0.5%
Recirculation Rate in Crystallizer	-1.0%	1.2%	-1.5%	1.9%	-2.4%	2.9%
Compressor Efficiencies	-2.3%	2.9%	-2.9%	3.5%	-3.6%	4.3%
Inlet Flowrate	-3.8%	4.5%	-3.7%	4.4%	-3.6%	4.2%

Table S47: Sensitivity of LCOW in Na_2SO_4 removal process using EDC

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Temperature Drop in Crystallization Tank	0.0%	0.0%	0.1%	-0.1%	0.0%	0.0%
RO Membrane Replacement Factor	0.1%	-0.1%	0.0%	0.0%	0.0%	0.0%
Crystallization Tank Retention Time	0.2%	-0.4%	0.3%	-0.2%	0.1%	-0.1%
Inlet Flowrate	-0.4%	0.3%	-0.1%	0.1%	0.0%	0.0%
IEM Replacement Factor	0.2%	-0.2%	0.4%	-0.4%	0.5%	-0.5%
Cost of Energy	1.7%	-1.7%	0.7%	-0.7%	0.2%	-0.2%
Lifetime	-1.7%	2.2%	-2.0%	5.2%	-4.5%	5.7%
Cost of IEM	4.9%	-4.9%	8.0%	-8.0%	9.5%	-9.5%
Inlet Salinity	6.8%	-6.7%	8.8%	-8.8%	9.7%	-9.7%
Current Density	-3.1%	4.1%	-6.8%	8.4%	-8.6%	10.5%
Crystal Yield	-5.7%	6.9%	-7.7%	9.4%	-8.7%	10.7%

Table S48: Sensitivity of LCOW in Na_2SO_4 removal process using MD+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Recirculation Rate in Crystallizer	-0.4%	0.4%	0.0%	0.2%	0.0%	0.0%
Compressor Efficiencies	-0.6%	0.7%	-0.1%	0.3%	0.0%	0.0%
Inlet Flowrate	-0.8%	0.9%	-0.4%	0.5%	-0.1%	0.2%
Lifetime	-1.1%	0.9%	-0.6%	1.5%	-1.3%	1.6%
Cost of Energy	7.1%	-7.1%	7.5%	-7.5%	7.3%	-7.3%
Inlet Salinity	0.1%	-0.8%	1.8%	-1.1%	14.6%	-10.6%
Inlet Temperature	-11.0%	15.6%	-16.1%	21.6%	-22.5%	37.6%
Recovery Rate in MD	5.4%	-6.1%	12.5%	-8.9%	186.7%	-27.9%

Table S49: Sensitivity of LCOW in Na_2SO_4 removal process using MD+C w/ WH

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Cost of Energy	0.7%	-0.7%	0.3%	-0.3%	0.0%	0.0%
Recirculation Rate in Crystallizer	-0.8%	0.9%	0.1%	0.5%	0.0%	0.0%
Compressor Efficiencies	-1.2%	1.4%	-0.1%	0.7%	-0.1%	0.1%
Inlet Flowrate	-1.7%	1.9%	-1.1%	1.2%	-0.4%	0.4%
Lifetime	-3.4%	2.9%	-2.3%	5.9%	-4.8%	6.0%
Inlet Salinity	0.0%	-1.5%	1.1%	-0.3%	13.4%	-9.6%
Inlet Temperature	-10.5%	15.3%	-16.1%	23.1%	-25.6%	45.3%
Recovery Rate in MD	2.1%	-3.7%	8.1%	-4.9%	176.7%	-25.0%

S.4.4.1.2. LCA

Table S50: Impacts of water treatment in a Na_2SO_4 removal process

	Cons. MVC+C	**Avg. MVC+C**	**Opt. MVC+C**	**Cons. EDC**	**Avg. EDC**	**Opt. EDC**	**Cons. MD+C**	**Avg. MD+C**	**Opt. MD+C**	**Cons MD+C w/WH**	**Avg. MD+C w/WH**	**Opt. MD+C w/WH**
Acidification (10^{-3} kg SO_2 eq/m^3)	47	32	26	24	23	21	1199	432	256	2	8	11
Carcinogenics (10^{-7} CTUh/m^3)	19	13	10	8	7	6	486	175	104	1	3	5
Ecotoxicity (10 CTUe/m^3)	19	13	11	11	11	10	481	173	102	1	3	5
Eutrophication (10^{-2} kg N eq/m^3)	18	12	10	6	6	5	457	165	97	1	3	4
Fossil Fuel Depletion (MJ surplus/m^3)	27	19	15	10	9	8	710	256	151	1	5	7
Global Warming Potential (kg CO_2 eq/m^3)	21	14	11	10	8	7	539	194	115	1	3	5
Non-carcinogenics (10^{-7} CTUh/m^3)	57	39	32	26	25	22	1472	531	314	2	9	14
Ozone Depletion (10^{-7} kg CFC-11 eq/m^3)	16	11	9	3370	1226	786	399	144	85	1	3	4
Respiratory Effects (10^{-3} kg PM2.5 eq/m^3)	79	54	43	26	25	20	2054	741	438	3	13	19
Smog (10^{-2} kg O_3 eq/m^3)	37	25	20	22	21	19	947	342	202	2	6	9
SEC (kWh/m^3)	44	30	24	13	12	10	1142	412	243	2	7	11

Table S51: Sensitivity of GWP in Na_2SO_4 removal process using MVC+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Salinity	-1.2%	1.2%	-0.1%	0.4%	1.9%	-1.9%
Recirculation Rate in Crystallizer	-3.0%	3.7%	-4.5%	5.5%	-6.2%	7.5%
Compressor Efficiencies	-9.0%	11.0%	-9.0%	11.0%	-9.1%	11.1%

Table S52: Sensitivity of GWP in Na_2SO_4 removal process using EDC

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of IEM	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Crystallization Tank Retention Time	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
RO Membrane Replacement Factor	0.6%	-0.6%	0.5%	-0.5%	0.5%	-0.5%
Temperature Drop in Crystallization Tank	0.0%	0.0%	0.9%	-0.9%	1.5%	-1.5%
IEM Replacement Factor	0.1%	-0.1%	0.4%	-0.4%	1.6%	-1.6%
Inlet Salinity	4.5%	-4.5%	4.6%	-4.6%	4.9%	-4.9%
Current Density	5.5%	-5.5%	4.5%	-4.4%	1.9%	-1.6%
Crystal Yield	-5.3%	6.5%	-4.9%	6.0%	-4.7%	5.8%

Table S53: Sensitivity of GWP in Na_2SO_4 removal process using MD+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Recirculation Rate in Crystallizer	-0.3%	0.3%	-0.1%	0.1%	0.0%	0.0%
Compressor Efficiencies	-0.4%	0.5%	-0.2%	0.2%	0.0%	0.0%
Inlet Salinity	0.0%	-0.1%	2.0%	-1.3%	15.4%	-11.3%
Inlet Temperature	-10.9%	15.2%	-15.8%	20.1%	-20.4%	32.3%
Recovery Rate in MD	7.2%	-7.2%	14.6%	-10.7%	193.0%	-29.6%

Table S54: Sensitivity of GWP in Na_2SO_4 removal process using MD+C w/ WH

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Temperature	0.0%	0.0%	-0.1%	0.0%	-0.1%	0.1%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	-0.9%	-0.9%
Recirculation Rate in Crystallizer	-6.1%	7.4%	-6.1%	7.4%	-5.0%	6.1%
Compressor Efficiencies	-9.1%	11.1%	-9.0%	11.0%	-8.9%	10.8%
Inlet Salinity	-4.2%	2.0%	-11.5%	12.1%	-24.3%	49.8%
Recovery Rate in MD	-14.3%	12.0%	-34.4%	37.1%	-30.3%	196.1%

S.4.4.2. NaCl Crystallization

S.4.4.2.1. TEA

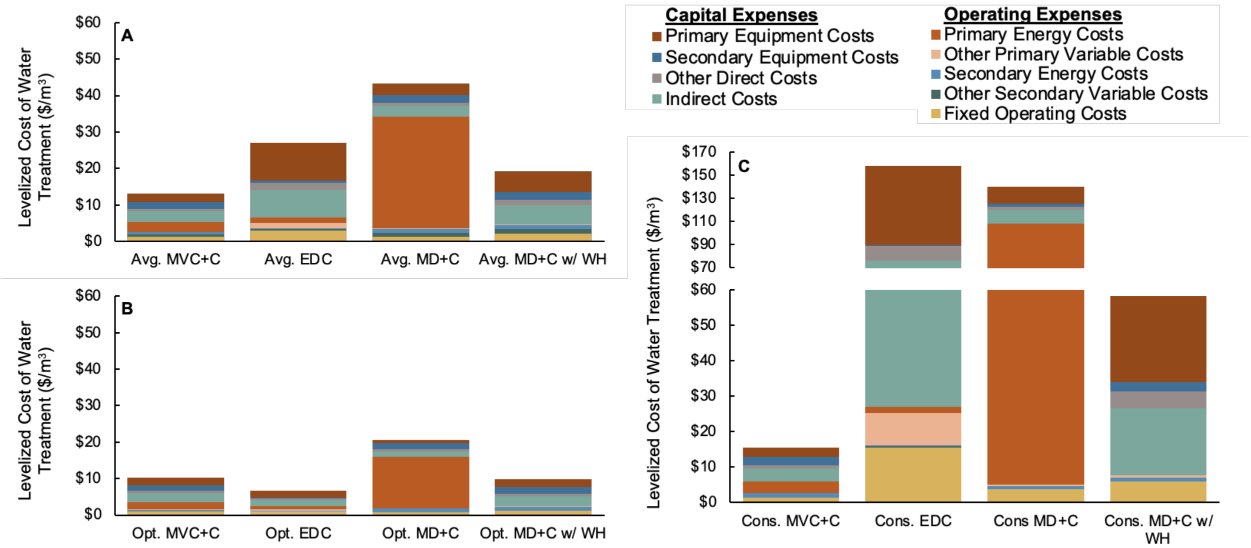

Figure S5: Levelized Cost of Treatment When Removing NaCl. Results are split into the A) average (Avg.), B) optimistic (Opt.), and C) conservative (Cons.) operation scenarios. The cost of electrodialytic crystallization (EDC) changes significantly between the operating scenarios, which displays the unpredictability of EDC performance, and the risk in developing full-scale EDC systems for zero liquid discharge desalination applications. Mechanical vapor compression paired with a crystallizer (MVC+C), membrane distillation paired with a crystallizer (MD+C), and MD+C when using waste heat (MD+C w/ WH) are the other technologies compared.

Table S55: Levelized cost of water in a NaCl removal process [$/m³]

ZLD Technology	Average Cost	Conservative Cost	Optimistic Cost
Total Cost (Sum of Capital and Operational Costs)			
MVC + Crystallizer	12.43	15.51	10.28
EDC	26.90	158.38	6.70
MD + Crystallizer	42.16	139.84	20.65
MD + Crystallizer w/ WH	18.01	52.32	9.88
Capital Cost (Equipment/All Other)			
MVC + Crystallizer	4.20/3.70	5.05/4.44	3.63/3.19
EDC	10.84/9.54	69.85/61.47	2.22/1.96
MD + Crystallizer	5.14/3.92	16.72/14.72	2.68/2.04
MD + Crystallizer w/ WH	7.75/6.82	26.97/23.72	4.00/3.52
Operational Cost (Energy/All Other)			
MVC + Crystallizer	3.30/1.23	4.55/1.47	2.39/1.07
EDC	1.08/4.70	2.24/24.82	1.19/1.33
MD + Crystallizer	31.61/1.49	104.06/4.33	15.09/0.84
MD + Crystallizer w/ WH	1.13/2.32	0.94/6.68	1.05/1.31

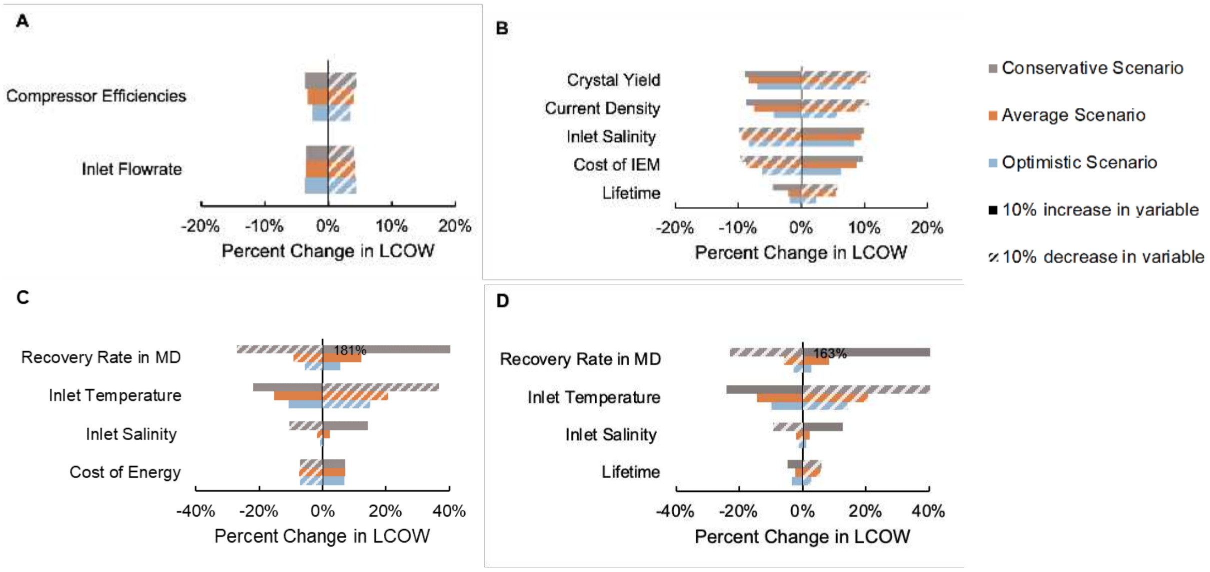

Figure S6: Sensitivity of levelized cost of water treatment (LCOW) with a 10% change of inputs when removing NaCl. A) mechanical vapor compression with a crystallizer (MVC+C), B) electrodialytic crystallization (EDC), C) membrane distillation with a crystallizer (MD+C), D) MD+C when using waste heat (MD+C w/ WH). A distinction has been made between increases and decreases to variables in the figure, which demonstrate either a positive (solid bar to the right) or a negative (dashed bar to the right) correlation with cost.

Table S56: Sensitivity of LCOW in NaCl removal process using MVC+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Recirculation Rate in Crystallizer	-0.3%	0.4%	-0.5%	0.6%	-0.8%	0.9%
Inlet Salinity	1.0%	-0.9%	0.9%	-0.9%	1.0%	-0.8%
Cost of Energy	1.8%	-1.8%	1.9%	-1.9%	2.0%	-2.0%
Inlet Flowrate	-3.7%	4.3%	-3.6%	4.2%	-3.4%	4.1%
Compressor Efficiencies	-2.5%	3.5%	-3.2%	4.0%	-3.6%	4.4%

Table S57: Sensitivity of LCOW in NaCl removal process using EDC

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Temperature Drop in Crystallization Tank	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
RO Membrane Replacement Factor	0.1%	-0.1%	0.0%	0.0%	0.0%	0.0%
Crystallization Tank Retention Time	0.1%	-0.2%	0.1%	-0.1%	0.0%	0.0%
Inlet Flowrate	-0.3%	0.2%	-0.1%	0.1%	0.0%	0.0%
IEM Replacement Factor	0.2%	-0.2%	0.4%	-0.4%	0.5%	-0.5%
Cost of Energy	1.6%	-1.6%	0.6%	-0.6%	0.1%	-0.1%
Lifetime	-1.8%	2.4%	-2.1%	5.4%	-4.5%	5.7%
Cost of IEM	6.3%	-6.3%	8.7%	-8.7%	9.7%	-9.7%
Inlet Salinity	8.3%	-8.3%	9.5%	-9.5%	9.9%	-9.9%
Current Density	-4.4%	5.7%	-7.5%	9.3%	-8.8%	10.7%
Crystal Yield	-7.0%	8.5%	-8.4%	10.2%	-8.9%	10.9%

Table S58: Sensitivity of LCOW in NaCl removal process using MD+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Recirculation Rate in Crystallizer	-0.4%	0.5%	-0.2%	0.3%	-0.1%	0.1%
Inlet Flowrate	-0.8%	0.9%	-0.5%	0.6%	-0.2%	0.2%
Compressor Efficiencies	-0.8%	0.9%	-0.4%	0.5%	-0.1%	0.1%
Lifetime	-1.1%	0.9%	-0.6%	1.7%	-1.3%	1.7%
Cost of Energy	7.0%	-7.0%	7.2%	-7.2%	7.2%	-7.2%
Inlet Salinity	0.7%	-0.8%	2.2%	-1.8%	14.4%	-10.5%
Inlet Temperature	-10.7%	15.2%	-15.4%	20.6%	-22.0%	36.7%
Recovery Rate in MD	5.6%	-5.6%	12.4%	-9.1%	180.7%	-27.0%

Table S59: Sensitivity of LCOW in NaCl removal process using MD+C w/ WH

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Cost of Energy	0.9%	-0.9%	0.6%	-0.6%	0.1%	-0.1%
Recirculation Rate in Crystallizer	-0.8%	0.9%	-0.5%	0.6%	-0.2%	0.2%
Inlet Flowrate	-1.7%	1.9%	-1.2%	1.3%	-0.5%	0.6%
Compressor Efficiencies	-1.6%	1.9%	-1.0%	1.2%	-0.3%	0.3%
Lifetime	-3.3%	2.8%	-2.2%	5.7%	-4.7%	6.0%
Inlet Salinity	1.2%	-1.3%	2.2%	-2.0%	12.8%	-9.2%
Inlet Temperature	-9.9%	14.4%	-14.4%	20.8%	-24.1%	42.7%
Recovery Rate in MD	2.9%	-3.0%	8.3%	-5.8%	163.1%	-23.0%

S.4.4.2.2. LCA

Table S60: Impacts of water treatment in a NaCl removal process

	Cons. MVC+C	Avg. MVC+C	Opt. MVC+C	Cons. EDC	Avg. EDC	Opt. EDC	Cons. MD+C	Avg. MD+C	Opt. MD+C	Cons MD+C w/WH	Avg. MD+C w/WH	Opt. MD+C w/WH
Acidification (10^{-3} kg SO_2 eq/m^3)	54	45	39	35	33	30	1207	439	261	10	15	17
Carcinogenics (10^{-7} CTUh/m^3)	22	18	16	12	11	10	490	178	106	4	6	7
Ecotoxicity (10 CTUe/m^3)	22	18	16	15	15	13	484	176	105	4	6	7
Eutrophication (10^{-2} kg N eq/m^3)	20	17	15	10	10	8	460	168	100	4	6	6
Fossil Fuel Depletion (MJ surplus/m^3)	32	26	23	16	15	13	714	260	155	6	9	10
Global Warming Potential (kg CO_2 eq/m^3)	24	20	17	17	13	11	542	197	117	5	6	8
Non-carcinogenics (10^{-7} CTUh/m^3)	66	55	48	39	37	33	1482	539	321	12	18	21
Ozone Depletion (10^{-7} kg CFC-11 eq/m^3)	18	15	13	6815	1799	814	402	146	87	3	5	6
Respiratory Effects (10^{-3} kg PM2.5 eq/m^3)	91	75	66	43	42	35	2068	753	447	17	25	29
Smog (10^{-2} kg O_3 eq/m^3)	43	35	31	30	29	26	954	347	206	8	12	13
SEC (kWh/m^3)	51	42	37	23	22	18	1150	419	249	10	14	16

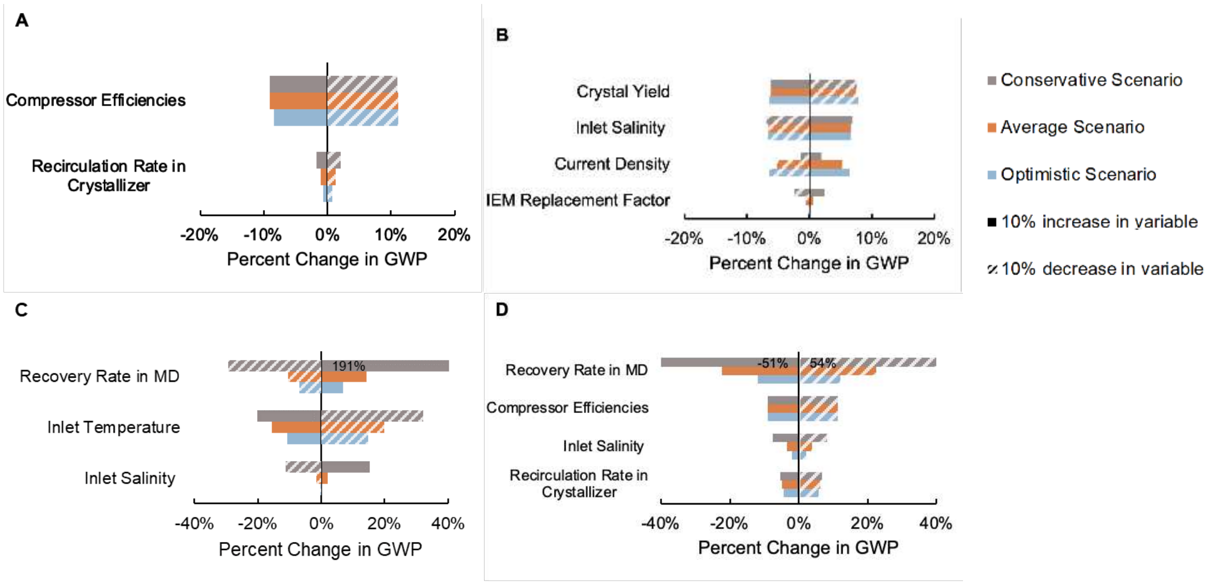

Figure S7: Sensitivity of levelized global warming potential with a 10% change of inputs when removing NaCl. A) mechanical vapor compression with a crystallizer (MVC+C), B) electrodialytic crystallization (EDC), C) membrane distillation with a crystallizer (MD+C), D) MD+C when using waste heat (MD+C w/ WH). A distinction has been made between increases and decreases to variables in the figure, which demonstrate either a positive (solid bar to the right) or a negative (dashed bar to the right) correlation with global warming potential (GWP).

Table S61: Sensitivity of GWP in NaCl removal process using MVC+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Recirculation Rate in Crystallizer	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Salinity	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	-0.9%	1.0%	-0.8%	0.9%	0.0%	0.4%
Inlet Flowrate	-0.6%	0.8%	-1.0%	1.2%	-1.7%	2.0%
Compressor Efficiencies	-8.5%	11.1%	-9.0%	11.2%	-9.1%	11.0%

Table S62: Sensitivity of GWP in NaCl removal process using EDC

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of IEM	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Crystallization Tank Retention Time	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
RO Membrane Replacement Factor	0.3%	-0.3%	0.2%	-0.2%	0.2%	-0.2%
Temperature Drop in Crystallization Tank	0.0%	0.0%	0.6%	-0.6%	0.9%	-0.9%
IEM Replacement Factor	0.2%	-0.2%	0.6%	-0.6%	2.4%	-2.4%
Current Density	6.5%	-6.4%	5.3%	-5.2%	1.9%	-1.4%
Inlet Salinity	6.6%	-6.6%	6.7%	-6.7%	6.9%	-6.9%
Crystal Yield	-6.4%	7.9%	-6.2%	7.5%	-6.2%	7.5%

Table S63: Sensitivity of GWP in NaCl removal process using MD+C

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Recirculation Rate in Crystallizer	-0.3%	0.4%	-0.2%	0.2%	0.0%	0.1%
Compressor Efficiencies	-0.6%	0.7%	-0.3%	0.4%	-0.1%	0.1%
Inlet Salinity	0.0%	-0.1%	2.0%	-1.4%	15.3%	-11.2%
Inlet Temperature	-10.7%	14.8%	-15.6%	19.8%	-20.2%	32.1%
Recovery Rate in MD	6.9%	-6.8%	14.2%	-10.4%	191.3%	-29.2%

Table S64: Sensitivity of GWP in NaCl removal process using MD+C w/ WH

	10% Increase to Optimistic Scenario	10% Decrease to Optimistic Scenario	10% Increase to Average Scenario	10% Decrease to Average Scenario	10% Increase to Conservative Scenario	10% Decrease to Conservative Scenario
Lifetime	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cost of Energy	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Flowrate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Inlet Temperature	0.0%	0.0%	-0.1%	0.0%	0.0%	0.0%
Recirculation Rate in Crystallizer	-4.5%	5.5%	-4.9%	6.0%	-5.2%	6.4%
Inlet Salinity	-1.9%	1.8%	-3.4%	3.4%	-7.6%	7.9%
Compressor Efficiencies	-9.1%	11.1%	-9.1%	11.1%	-9.0%	11.1%
Recovery Rate in MD	-11.8%	11.8%	-22.3%	22.4%	-51.1%	54.0%

S.5. Stakeholder Influenced Triple Bottom Line Tradeoffs Results

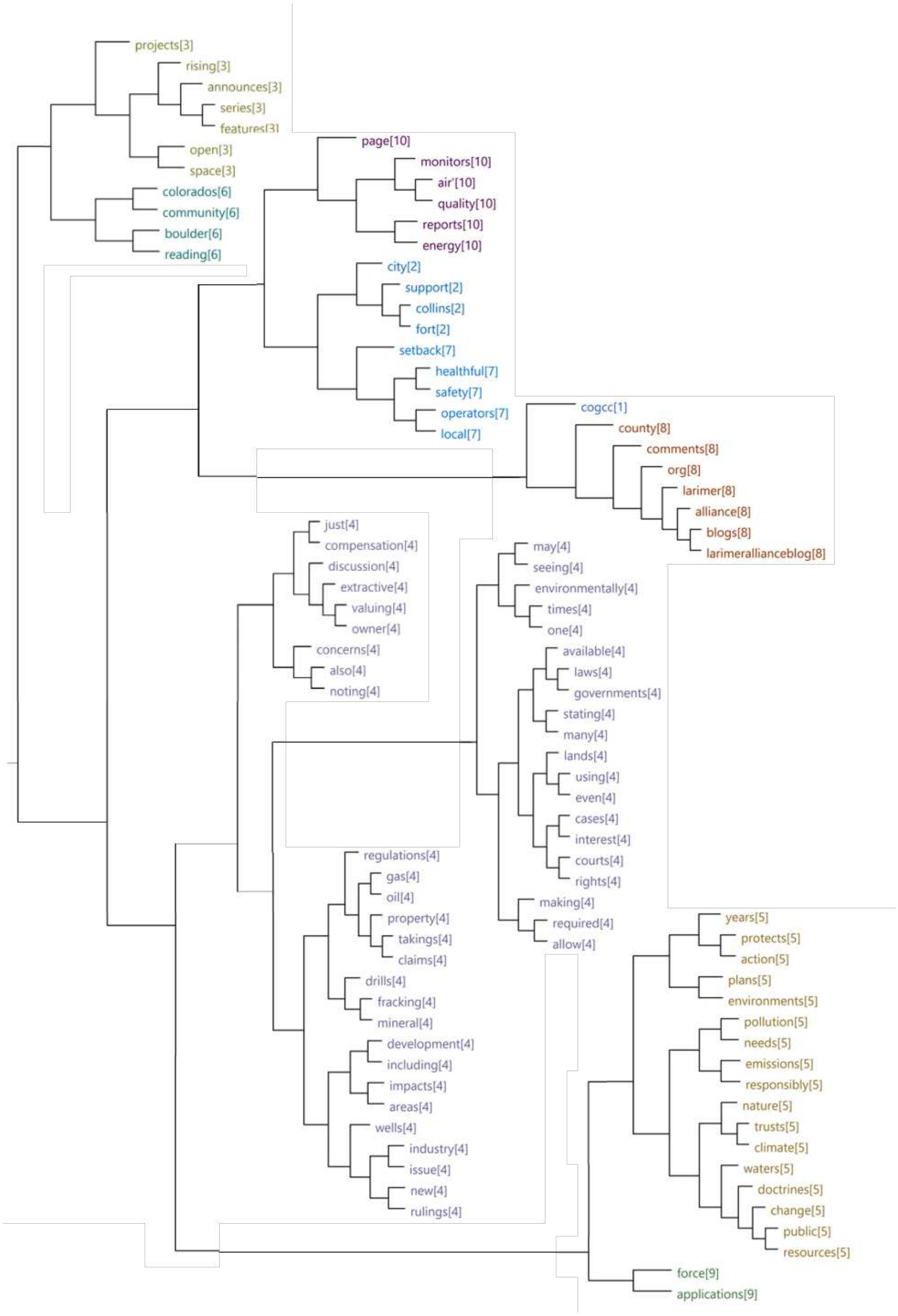

Figure S8: Cluster of top 100 frequent words in community written communications. The words are clustered into 10 major groups, denoted by their bracketed numbers.

Table S65: Top 25 words from each Stakeholder group

Community		**Researchers**	
Keyword	**Comments/Context**	**Keyword**	**Comments/Context**
Colorado	Represented under the modified keyword “Local”.	Gas	Represented under the modified keyword “Oil & Gas”.
Gas	Represented under the modified keyword “Oil & Gas”.	Oil	Represented under the modified keyword “Oil & Gas”.
Oil	Represented under the modified keyword “Oil & Gas”.	Waters	Directly transitioned to a DPSIR keyword.
Fracking	Represented under the modified keyword “Hydraulic Fracturing”.	Fracturing	Represented under the modified keyword “Hydraulic Fracturing”.
Taking	Directly transitioned to a DPSIR keyword.	Energy	Directly transitioned to a DPSIR keyword.
Public	Directly transitioned to a DPSIR keyword.	Hydraulic	Represented under the modified keyword “Hydraulic Fracturing”.
Stating	"stating" and "many" are branched closely to "governments" and "laws" and "available". These associated words indicate that the majority of "state", "stating", "states", etc. are synonymized with "said", rather than a physical state of being. Directly transitioned to a DPSIR keyword.	Methane	Directly transitioned to a DPSIR keyword.
County	County does not provide any additional information beyond the keywords of “Local”, “Public” and “Community”.	Model	Directly transitioned to a DPSIR keyword.
Larimer	Represented under the modified keyword “Local”.	Emissions	Directly transitioned to a DPSIR keyword.
Regulation	Directly transitioned to a DPSIR keyword.	Hydrate	Typically refers to the clathrate hydrates formed within water-oil mixtures. Directly transitioned to a DPSIR keyword.
New	“New” is associated with "Rulings" in the word association map. In a further step, they are associated with "issue" and "industry". It is my interpretation that “new” can be captured by the keywords of “regulations” and “courts” withing this context.	Shale	Directly transitioned to a DPSIR keyword.
Rising	“Rising” is a biased word because of Colorado Rising. As such, it is captured under “community organization.”	Natural	“Natural” is primarily originating from “Natural Gas.” Replaced with the keyword of “Natural Gas” in DPSIR.
Community	Directly transitioned to a DPSIR keyword.	Flows	Directly transitioned to a DPSIR keyword.
Court	Directly transitioned to a DPSIR keyword.	Produced	“Produced” is primarily originating from “Produced Water”, Replaced with the keyword of “Produced Water” in DPSIR.
Property	Directly transitioned to a DPSIR keyword.	Policy	Directly transitioned to a DPSIR keyword.
May	Could relate to a sense of uncertainty in the community. Directly transitioned to a DPSIR keyword.	Carbon	Directly transitioned to a DPSIR keyword.
Law	Directly transitioned to a DPSIR keyword.	Development	Represented under the modified keywords “Oil & Gas” and “Energy”.
Air	Directly transitioned to a DPSIR keyword.	Unconventional	Represented under the modified keyword “Hydraulic Fracturing”.
Rights	Directly transitioned to a DPSIR keyword.	Colorado	Represented under the modified keyword “Local”.
Alliance	Replaced with the keyword of “Community Organizations” in DPSIR: Alliance is a biased word because of Larimer Alliance. However, it, combined with other organizations deserve a representation in the DPSIR.	Fracking	Represented under the modified keyword “Hydraulic Fracturing”.
Industry	Directly transitioned to a DPSIR keyword.	Analysis	Directly transitioned to a DPSIR keyword.
Government	Directly transitioned to a DPSIR keyword.	Reservoir	Directly transitioned to a DPSIR keyword.
Health	Directly transitioned to a DPSIR keyword.	Environment	Directly transitioned to a DPSIR keyword.
Operators	Represented under the keyword “Industry.”	Organic	“Organic” is primarily originating from “Volatile Organic Carbon”, or VOCs. As such, it is replaced with the modified keyword of “VOCs”
Protect	Directly transitioned to a DPSIR keyword.	Carbon Dioxide	Represented under the keyword “Carbon.”

Table S66: Stakeholder-sourced keywords and their EH-DPSIR elements, and PW-relevant elements.

Source	**Modified Keyword**	**PW-Relevant Element**	**DPSIR**	**DPSIR Category**	**Element**	**Sub-Element**	**Indicator**
Community	Air	Air Quality	State	Environmental State	Abiotic	Physical & Chemical Environment	Air Quality
Community	Air	Atmospheric Emissions	Pressure	Environmental Pressure	Discharges	Atmospheric Discharges	Atmospheric Emissions
Community	Air	Emissions Regulations	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Air Quality Criteria	SKIP - RESPONSE
Community	Air	Emissions Regulations	Response	Infrastructural Policies	Economic Markets & policies	Carbon Credits	SKIP - RESPONSE
Community	Air	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Air, Soil, & Water Monitoring	SKIP - RESPONSE
Community	Air	Public Health	State	Human State	Individuals	Body Systems	Public Health
Researchers	Analysis	Access to Education & Information	Driver	Economic Driver	Culture	Education & Information	Access to Education & Information
Researchers	Analysis	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Develop & Manage an Ecosystems Database		SKIP - RESPONSE
Researchers	Analysis	System Models	Response	Ecosystem Monitoring & Restoration			SKIP - RESPONSE
Researchers	Analysis	System Models	Response	Security & Public Administration Policies	Decision Support		SKIP - RESPONSE
Researchers	Analysis	System Models	Response	Valuation			SKIP - RESPONSE
Researchers	Carbon	Atmospheric Emissions	Pressure	Environmental Pressure	Discharges	Atmospheric Emissions	Atmospheric Emissions
Researchers	Carbon	Emissions Regulations	Response	Infrastructural Policies	Economic Markets and Policies	Carbon Credits	SKIP - RESPONSE
Researchers	Carbon	Global Warming Potential	State	Environmental State	Abiotic	Physical & Chemical State	GHG Emissions
Community	Community	Access to Education & Information	Driver	Social Drivers	Equity	Access to Education	Access to Education & Information
Community	Community	Access to Healthcare	Driver	Social Drivers	Equity	Access to healthcare	Access to Healthcare
Community	Community	Access to Jobs	Driver	Social Drivers	Equity	Access to Jobs	Access to Jobs
Community	Community	Access to Jobs	Impact	Human Well-being	Economic Prosperity	Ability to Work	Access to Jobs
Community	Community	Community Involvement	Driver	Social Drivers	Social Relations	Social Group	Community Involvement
Community	Community	Community Livability	State	Human State	Communities		Community Livability
Community	Community	Cultural Well-Being	Driver	Social Drivers	Abiotic State	Community Identity	Cultural Well-being
Community	Community	Cultural Well-Being	Driver	Social Drivers	Abiotic State	Ethnic Identity	Cultural Well-being
Community	Community	Cultural Well-Being	Driver	Social Drivers	Abiotic State	Religious Identity	Cultural Well-being
Community	Community	Cultural Well-Being	Impact	Human Well-being	Cultural & Social Well-being	Community Vibrancy	Cultural Well-being
Community	Community	Cultural Well-Being	Impact	Human Well-being	Cultural & Social Well-being	Sense of Belonging	Cultural Well-being
Community	Community	Cultural Well-Being	State	Human State	Communities	Population Demographics	Cultural Well-being
Community	Community	Cultural Well-Being	State	Human State	Communities	Population Demographics	Cultural Well-being
Community	Community	Cultural Well-Being	State	Human State	Communities	Population Demographics	Cultural Well-being
Community	Community	Cultural Well-Being	State	Human State	Communities	Population Demographics	Cultural Well-being
Community	Community	Cultural Well-Being	State	Human State	Communities	Population Demographics	Cultural Well-being
Community	Community	Cultural Well-Being	State	Human State	Communities	Population Distribution	Cultural Well-being
Community	Community	Economic Prosperity	Impact	Human Well-being	Economic Prosperity	Income	Economic Prosperity
Community	Community	Economic Prosperity	Impact	Human Well-being	Economic Prosperity	Productivity	Economic Prosperity
Community	Community	Public Health	State	Human State	Communities	Public Health Status	Public Health
Community	Community	Representation of Stakeholders	Driver	Social Drivers	Governance	Role of Decision Makers	Community Livability
Community	Community	Value of Community	Impact	Ecosystem Services	Cultural Services	Existence Value & Sense of Place	Community Livability
Community	Community Organizations	Community Involvement	Driver	Economic Driver	Culture	Social Organizations	Community Involvement
Community	Community Organizations	Community Involvement	Driver	Social Drivers	Social Relations	Social Group	Community Involvement

Community	Community Organizations	Education	Response	Cultural Policies	Environmental Education & Outreach		SKIP - RESPONSE
Community	Community Organizations	Environmental Policy	Response	Ecosystem Monitoring & Restoration			SKIP - RESPONSE
Community	Community Organizations	Stakeholder Involvement	Response	Cultural Policies	Collaboration & Partnering		SKIP - RESPONSE
Community	Community Organizations	Stakeholder Involvement	Response	Security & Public Administration Policies	Collaboration & Partnering		SKIP - RESPONSE
Community	Court	Administrative Action	Driver	Economic Driver	Security	Public Administration	Administrative Action
Researchers	Emissions	Atmospheric Emissions	Pressure	Environmental Pressure	Discharges	Atmospheric Emissions	Atmospheric Emissions
Researchers	Emissions	Discharge Regulations	Response	Discharge Limitations			SKIP - RESPONSE
Researchers	Emissions	Emissions Regulations	Response	Infrastructural Policies	Economic Markets and Policies	Carbon Credits	SKIP - RESPONSE
Researchers	Emissions	Industry Liability	Response	Infrastructural Policies	Corporate Responses		SKIP - RESPONSE
Researchers	Energy	Resource Management	Response	Resource Use Management	Sustainable Resource Use		SKIP - RESPONSE
Researchers	Energy	Technological Improvements	Response	Technology Innovations			SKIP - RESPONSE
Researchers	Environment	Administrative Action	Driver	Economic Driver	Security	Public Administration	Administrative Action
Researchers	Environment	Carbon Cycling	Impact	Ecosystem Services			Environmental Health
Researchers	Environment	Emissions Regulations	Response	Infrastructural Policies	Economic Markets and Policies	Carbon Credits	SKIP - RESPONSE
Researchers	Environment	Environmental Health	State	Environmental State			Environmental Health
Researchers	Environment	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Environmental Monitoring, Mapping, & Scientific Research	SKIP - RESPONSE
Researchers	Environment	Industry Liability	Response	Infrastructural Policies	Corporate Responses		SKIP - RESPONSE
Researchers	Environment	Natural Water Cycles	Impact	Ecosystem Services	Regulating Services		Natural Water Cycles
Researchers	Environment	System Models	Response	Ecosystem Monitoring & Restoration			SKIP - RESPONSE
Researchers	Environment	System Models	Response	Security & Public Administration Policies	Decision Support		SKIP - RESPONSE
Researchers	Flow	Resource Management	State	Environmental State	Abiotic	Physical & Chemical Environment	Resource Management
Researchers	Flow	Water Preservation	Response	Discharge Limitations	Hydrologic Management		SKIP - RESPONSE
Researchers	Flow	Water Quality	State	Environmental State			SKIP - RESPONSE
Community	Government	Cultural Protections	Response	Cultural Policies			SKIP - RESPONSE
Community	Government	Discharge Regulations	Response	Discharge Limitations			SKIP - RESPONSE
Community	Government	Environmental Policy	Response	Ecosystem Monitoring & Restoration			SKIP - RESPONSE
Community	Government	Equitable Burdens	Driver	Social Drivers	Equity		Equitable Burdens
Community	Government	Representation of Stakeholders	Driver	Social Drivers	Governance		Community Livability
Community	Government	Resource Use	Driver	Economic Driver	Utilities	Water	Resource Use
Community	Health	Access to Healthcare	Impact	Human Well-being	Health & Safety		Access to Healthcare
Community	Health	Public Health	Driver	Economic Driver	Security	Public Administration	Public Health
Community	Health	Public Health	State	Human State	Communities	Public Health Status	Public Health
Community	Health	Public Health	State	Human State	Individuals	Body Systems	Public Health
Community	Health	Public Health	Response	Valuation	Index of Human Well-being		SKIP - RESPONSE
Community	Industry	Atmospheric Emissions	Pressure	Environmental Pressure	Discharges	Atmospheric Emissions	Atmospheric Emissions
Community	Industry	Chemical Use	Pressure	Environmental Pressure	Discharges	Applied Chemicals	Chemical Use
Community	Industry	Clean Water Access	Impact	Ecosystem Services	Provisioning Services	Water Resources	Resource Management
Community	Industry	Discharge Regulations	Response	Discharge Limitations	Chemical Use Regulations		SKIP - RESPONSE
Community	Industry	Economic Prosperity	Response	Valuation	Monetary Valuation		SKIP - RESPONSE
Community	Industry	Industry Liability	Response	Infrastructural Policies	Corporate Response		SKIP - RESPONSE
Community	Industry	Natural Water Cycles	Impact	Ecosystem Services	Regulating Services	Water Regulation	Natural Water Cycles

Community	Industry	Political Incentive	Response	Security & Public Administration Policies	Political Pressure		SKIP - RESPONSE
Community	Industry	Resource Management	Response	Resource Use Management			SKIP - RESPONSE
Community	Industry	Stakeholder Involvement	Response	Security & Public Administration Policies	Collaboration & Partnering		SKIP - RESPONSE
Community	Industry	Technological Improvements	Response	Technological Innovation			SKIP - RESPONSE
Community	Industry	Transportation Requirements	Driver	Economic Driver	Transportation	Land & Air Transportation	Transportation Requirements
Community	Law	Cultural Protections	Response	Cultural Policies			SKIP - RESPONSE
Community	Law	Discharge Regulations	Response	Discharge Limitations			SKIP - RESPONSE
Community	Law	Resource Management	Response	Resource Use Management			SKIP - RESPONSE
Both	Local	Community Involvement	Driver	Social Drivers	Social Relations	Social Group	Community Involvement
Both	Local	Community Livability	State	Human State	Communities		Community Livability
Both	Local	Cultural Protections	Response	Cultural Policies			SKIP - RESPONSE
Both	Local	Cultural Well-Being	State	Human State	Communities	Population Distribution	Cultural Well-being
Both	Local	Economic Prosperity	Impact	Human Well-being	Economic Prosperity		Economic Prosperity
Both	Local	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Biological Monitoring & Restoration		SKIP - RESPONSE
Both	Local	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration		SKIP - RESPONSE
Both	Local	Equitable Burdens	Driver	Social Drivers	Equity		Equitable Burdens
Both	Local	Public Health	State	Human State	Communities	Public Health Status	Public Health
Both	Local	Representation of Stakeholders	Driver	Social Drivers	Governance	Role of Decision Makers	Community Livability
Both	Local	Stakeholder Involvement	Response	Culture	Collaboration & Partnering	Utilizing Local Knowledge	SKIP - RESPONSE
Both	Local	Value of Community	Impact	Human Well-being	Cultural & Social Well-being	Community Vibrancy	Community Livability
Community	May	Cultural Well-Being	Impact	Human Well-being	Cultural & Social Well-being		Cultural Well-being
Community	May	Economic Prosperity	Impact	Human Well-being	Economic Prosperity		Economic Prosperity
Community	May	Equitable Burdens	Driver	Social Drivers	Equity		Equitable Burdens
Community	May	Public Security	Driver	Economic Driver	Security		Community Livability
Community	May	Value of Community	Impact	Human Well-being	Health & Safety		Community Livability
Researchers	Methane	Atmospheric Emissions	Pressure	Environmental Pressure	Discharges	Atmospheric Emissions	Atmospheric Emissions
Researchers	Model	Environmental Health	State	Environmental State			Environmental Health
Researchers	Model	Produced Water Research	Driver	Economic Driver	Culture	Education & Information	Produced Water Research
Researchers	Model	System Models	Response	Security & Public Administration Policies	Decision Support	Decision Support Tools	SKIP - RESPONSE
Both	Oil and Gas	Economic Prosperity	Driver	Economic Driver			Economic Prosperity
Both	Oil and Gas	Oil & Gas Industry	Driver	Economic Driver	Food and Raw Materials	Oil and Gas Industry	Economic Prosperity
Researchers	Policy	Discharge Regulations	Response	Discharge Limitations	Chemical Use Regulations		SKIP - RESPONSE
Researchers	Policy	Emissions Regulations	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Air Quality Criteria	SKIP - RESPONSE
Researchers	Policy	Emissions Regulations	Response	Infrastructural Policies	Economic Markets and Policies	Carbon Credits	SKIP - RESPONSE
Researchers	Policy	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Air, Water, & Soil Monitoring	SKIP - RESPONSE
Researchers	Policy	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Environmental Monitoring, Mapping, & Scientific Research	SKIP - RESPONSE
Researchers	Policy	Equitable Policies	Response	Cultural Policies	Equity Policies		SKIP - RESPONSE
Researchers	Policy	Stakeholder Involvement	Response	Cultural Policies	Collaboration & Partnering	Utilizing Local Knowledge	SKIP - RESPONSE
Researchers	Policy	Waste Management Strategies	Response	Infrastructural Policies	Utility Policies	Waste Management Policies	SKIP - RESPONSE
Researchers	Policy	Water Regulation	Response	Discharge Limitations	Hydrologic Management		SKIP - RESPONSE

Researchers	Policy	Water Regulation	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Physical & Chemical Water Quality Criteria	SKIP - RESPONSE
Researchers	Policy	Water Regulation	Response	Resource Use Management	Clean Water Act		SKIP - RESPONSE
Researchers	Produced Water	Clean Water Access	Impact	Ecosystem Services	Provisioning Services	Water Resources	Resource Management
Researchers	Produced Water	Discharge Regulations	Response	Discharge Limitations	Chemical Use Regulations		SKIP - RESPONSE
Researchers	Produced Water	Environmental Policy	Response	Discharge Limitations	Environmental Monitoring & Restoration	Air, Water, & Soil Monitoring	SKIP - RESPONSE
Researchers	Produced Water	Environmental Policy	Response	Discharge Limitations	Environmental Monitoring & Restoration	Remediation	SKIP - RESPONSE
Researchers	Produced Water	Natural Water Cycles	Impact	Ecosystem Services	Regulating Services	Water Regulation	Natural Water Cycles
Researchers	Produced Water	Produced Water Discharge	Driver	Economic Driver	Utilities	Waste Management	Produced Water Discharge
Researchers	Produced Water	Produced Water Discharge	Pressure	Environmental Pressure	Discharges	Waterborne Discharges	Produced Water Discharge
Researchers	Produced Water	Produced Water Discharge	Pressure	Environmental Pressure	Discharges	Waterborne Discharges	Produced Water Discharge
Researchers	Produced Water	Water Regulation	Response	Discharge Limitations	Environmental Monitoring & Restoration	Physical & Chemical Water Quality Criteria	SKIP - RESPONSE
Community	Property	Environmental Health	State	Environmental State			Environmental Health
Community	Property	Environmental Policy	Response	Ecosystem Monitoring & Restoration			SKIP - RESPONSE
Community	Property	Property Value	Driver	Economic Driver	Finance & Insurance		Property Value
Community	Protect	Environmental Policy	Response	Ecosystem Monitoring & Restoration	Environmental Monitoring & Restoration	Remediation	SKIP - RESPONSE
Community	Protect	Resource Management	Response	Resource Use Management			SKIP - RESPONSE
Community	Public	Public Health	State	Human State	Communities	Public Health Status	Public Health
Community	Public	Public Security	Driver	Economic Driver	Security	Public Administration	Community Livability
Community	Public	Stakeholder Involvement	Response	Security & Public Administration Policies	Collaboration & Partnering		SKIP - RESPONSE
Community	Regulation	Discharge Regulations	Response	Discharge Limitations			SKIP - RESPONSE
Researchers	Reservoir	Clean Water Access	Impact	Ecosystem Services	Provisioning Services	Water Resources	Resource Management
Researchers	Reservoir	Clean Water Access	Impact	Ecosystem Services	Supporting Services	Water Cycling	Resource Management
Researchers	Reservoir	Water Preservation	Response	Discharge Limitations	Hydrologic Management		SKIP - RESPONSE
Community	Rights	Access to Jobs	Impact	Human Well-being	Economic Prosperity	Ability to Work	Access to Jobs
Community	Rights	Equitable Burdens	Driver	Social Drivers	Equity		Equitable Burdens
Community	Rights	Physical & Mental Well-Being	Impact	Human Well-being	Health & Safety		Public Health
Community	Rights	Public Health	State	Human State	Individuals	Body Systems	Public Health
Community	Rights	Representation of Stakeholders	Driver	Social Drivers	Governance	Role of Decision Makers	Community Livability
Community	Rights	Value of Community	Impact	Human Well-being	Cultural & Social Well-being		Community Livability
Community	Stating	Cultural Well-Being	Impact	Human Well-being	Cultural & Social Well-being		Cultural Well-being
Community	Taking	Administrative Action	Driver	Economic Driver	Security	Public Administration	Administrative Action
Community	Taking	Clean Water Access	Impact	Ecosystem Services	Provisioning Services	Water Resources	Resource Management
Community	Taking	Equitable Burdens	Driver	Social Drivers	Equity		Equitable Burdens
Community	Taking	Representation of Stakeholders	Driver	Social Drivers	Governance	Role of Decision Makers	Representation of Stakeholders
Community	Taking	Stakeholder Involvement	Response	Cultural Policies	Collaboration & Partnering		SKIP - RESPONSE
Community	Taking	Stakeholder Involvement	Response	Security & Public Administration Policies	Collaboration & Partnering		SKIP - RESPONSE
Community	Taking	Value of Community	Impact	Human Well-being	Cultural & Social Well-being		Community Livability
Researchers	VOCs	Air Quality	State	Environmental State	Abiotic	Physical & Chemical Environment	Air Quality
Researchers	VOCs	Atmospheric Emissions	Pressure	Environmental Pressure	Discharges	Atmospheric Emissions	Atmospheric Emissions
Researchers	Water	Access to Clean Water	Driver	Economic Driver			Access to Clean Water

Researchers	Water	Clean Water Access	Impact	Ecosystem Services	Provisioning Services	Water Resources	Resource Management
Researchers	Water	Clean Water Access	Impact	Ecosystem Services	Provisioning Services	Water Resources	Resource Management
Researchers	Water	Clean Water Access	Impact	Ecosystem Services	Supporting Services	Water Cycling	Resource Management
Researchers	Water	Environmental Policy	Response	Discharge Limitations	Environmental Monitoring & Restoration	Air, Water, & Soil Monitoring	SKIP - RESPONSE
Researchers	Water	Natural Water Cycles	Impact	Ecosystem Services	Regulating Services	Water Regulation	Natural Water Cycles
Researchers	Water	Resource Management	State	Environmental State	Abiotic	Physical & Chemical Environment	Resource Management
Researchers	Water	Resource Use	Driver	Economic Driver	Utilities	Water	Resource Use
Researchers	Water	Resource Use Decisions	Response	Resource Use Management	Sustainable Resource Use		SKIP - RESPONSE
Researchers	Water	Water Preservation	Response	Discharge Limitations	Hydrologic Management		SKIP - RESPONSE
Researchers	Water	Water Quality	State	Environmental State			Water Quality
Researchers	Water	Water Regulation	Response	Discharge Limitations	Environmental Monitoring & Restoration	Physical & Chemical Water Quality Criteria	SKIP - RESPONSE
Researchers	Water	Water Regulation	Response	Resource Use Management	Clean Water Act		SKIP - RESPONSE
Researchers	Water	Waterborne Discharges	Pressure	Environmental Pressure	Discharges	Waterborne Discharges	Water Quality

Table S67: Modified keywords that lead to each PW-relevant element, and their DPSIR categorization.

PW-Relevant Element	Modified Keywords (Stakeholder Source: C=Community, R=Researchers, B=Both)	DPSIR
Access to Clean Water	Water (R)	Driver
Access to Education & Information	Analysis (R), Community (C)	Driver
Access to Healthcare	Community (C), Health (C)	Driver, Impact
Access to Jobs	Community (C), Rights (C)	Driver, Impact
Administrative Action	Court (C), Environment (R), Taking (C)	Driver
Air Quality	Air (C), VOCs (R)	State
Atmospheric Emissions	Air (C), Carbon (R), Emissions (R), Industry (C), Methane (R), VOCs (R)	Pressure
Carbon Cycling	Environment (R)	Impact
Chemical Use	Industry (C)	Pressure
Clean Water Access	Industry (C), Produced Water (R), Reservoir (R), Taking (C), Water (R), Water (R)	Impact
Community Involvement	Community (C), Community Organizations (C), Local (B)	Driver
Community Livability	Community (C), Local (B)	State
Cultural Protections	Government (C), Law (C), Local (B)	Response
Cultural Well-Being	Community (C), Local (B), May (C), Stating (C)	Driver, Impact, State
Discharge Regulations	Emissions (R), Government (C), Industry (C), Law (C), Policy (R), Produced Water (R), Regulation (C)	Response
Economic Prosperity	Community (C), Industry (C), Local (B), May (C), Oil and Gas (B)	Response, Impact, Driver
Education	Community Organizations (C)	Response
Emissions Regulations	Air (C), Carbon (R), Emissions (R), Environment (R), Policy (R)	Response
Environmental Health	Environment (R), Model (R), Property (C)	State
Environmental Policy	Air (C), Analysis (R), Community Organizations (C), Environment (R), Government (C), Local (B), Policy (R), Produced Water (R), Property (C), Protect (C), Water (R)	Response
Equitable Burdens	Government (C), Local (B), May (C), Rights (C), Taking (C)	Driver
Equitable Policies	Policy (R)	Response
Global Warming Potential	Carbon (R)	State
Industry Liability	Emissions (R), Environment (R), Industry (C)	Response
Natural Water Cycles	Environment (R), Industry (C), Produced Water (R), Water (R)	Impact
Oil & Gas Industry	Oil and Gas (B)	Driver
Physical & Mental Well-Being	Rights (C)	Impact
Political Incentive	Industry (C)	Response
Produced Water Discharge	Produced Water (R)	Driver, Pressure
Produced Water Research	Model (R)	Driver
Property Value	Property (C)	Driver
Public Health	Air (C), Community (C), Health (C), Local (B), Public (C), Rights (C)	Driver, Response, State
Public Security	May (C), Public (C)	Driver
Representation of Stakeholders	Community (C), Government (C), Local (B), Rights (C), Taking (C)	Driver,
Resource Management	Energy (R), Flow (R), Industry (C), Law (C), Protect (C), Water (R)	Response, State
Resource Use	Government (C), Water (R)	Driver
Resource Use Decisions	Water (R)	Response
Stakeholder Involvement 6	Community Organizations (C), Industry (C), Local (B), Policy (R), Public (C), Taking (C)	Response
System Models	Analysis (R), Environment (R), Model (R)	Response
Technological Improvements	Energy (R), Industry (C)	Response
Transportation Requirements	Industry (C)	Driver
Value of Community	Community (C), Local (B), May (C), Rights (C), Taking (C)	Impact
Waste Management Strategies	Policy (R)	Response
Water Preservation	Flow (R), Reservoir (R), Water (R)	Response
Water Quality	Flow (R), Water (R)	State
Water Regulation	Policy (R), Produced Water (R), Water (R)	Response
Waterborne Discharges	Water (R)	Pressure

Table S68: Indicators and possible metrics identified through DPSIR. This table also discusses why or why not an indicator is included in the analysis.

Indicator	PW-Relevant Element	DPSIR	DPSIR Category	Possible Indicator Metric	Included?	Why?
Access to Clean Water	Access to Clean Water	Driver	Economic Driver	Water quality (number of discharges that threaten existing water sources, treatment efficacy, natural water source constituent changes), distance to natural clean water source, water treatment intensity for utilities	N	Included as part of the community livability indicator. Information not readily available.
Access to Education & Information	Access to Education & Information	Driver	Social Drivers	Number of industry sponsored information events, number government sponsored information events, number of mailed informational items, number of blogs, publications, and websites available to the public	N	Included as part of the equitable burdens indicator. Information not readily available.
		Driver	Economic Driver			
Access to Healthcare	Access to Healthcare	Driver	Social Drivers	Distance to major healthcare facilities, healthcare quality	N	Included as part of the public health indicator.
		Impact	Human Well-being			
Access to Jobs	Access to Jobs	Driver	Social Drivers	Number of jobs being generated for technology operation and support	N	Systems are not modelled far enough to estimate necessary jobs to support each technology.
		Impact	Human Well-being			
Administrative Action	Administrative Action	Driver	Economic Driver	Number of governmental interventions, number of interventions to support public health, number of environmental interventions, treatment efficacy (amount of contaminants removed), treatment reliability (necessary allocations to maintenance)	N	Information not readily available.
Air Quality	Air Quality	State	Environmental State	Atmospheric emissions (GHG emissions, VOCs emitted), air quality index measurements	N	Partially included as part of the environmental health indicator. Information on air quality index measurements is not readily available.
Atmospheric Emissions	Atmospheric Emissions	Pressure	Environmental Pressure	GHG emissions (Methane emissions, carbon emission, NOx emissions), VOCs emitted	N	Included as part of the environmental health indicator. Data available from Life Cycle Assessments. VOCs are approximated by the smog effects of the system. The methodology used by TRACI states that VOCs are a necessary precursor to smog.
Chemical Use	Chemical Use	Pressure	Environmental Pressure	Amount of chemical products used	N	Included as part of the air quality indicator. Information available in Life Cycle Inventory, however it is better interpreted through the TRACI impacts which include those from chemical use.
Community Involvement	Community Involvement	Driver	Economic Driver	Number of O&G based groups in the community, percentage of community-generated articles mentioning produced water	N	

		Driver	Social Drivers			Irrelevant to this comparison, as community interest in PW management will not change with the technologies being used.
Community Livability	Community Livability	State	Human State	Cultural well-being (sense of involvement, sense of belonging, sense of community, sense of identity), economic prosperity (available jobs, housing costs, per capita income), sense of security (measured using Likert scale with surveys), equitable burdening (Stakeholder involvement, access to healthcare, burdened population distributions, equitable access to education & information, equitably-based policies), aesthetics (natural landscape retention, sightlines retention, wildlife retention), number of trucks driving through, access to clean water (water quality, distance to natural clean water source, water treatment intensity for utilities), heat vulnerability index	N	Information not readily available.
	Public Security	Driver	Economic Driver			
	Value of Community	Impact	Ecosystem Services			
		Impact	Human Well-being			
Cultural Well-being	Cultural Well-Being	Driver	Social Drivers	Community sense of involvement, sense of belonging, sense of community, sense of identity, measured using Likert scale with surveys	N	Information not readily available.
		Impact	Human Well-being			
		State	Human State			
Economic Prosperity	Economic Prosperity	Impact	Human Well-being	Technology costs, operation costs, transportation costs, insurance costs, per capita income, access to jobs (number of jobs being generated for technology operation and support)	Y	Have technology capital and operational costs, which include electricity, chemical, maintenance, and insurance costs.
	Oil & Gas Industry	Driver	Economic Driver			
Environmental Health	Environmental Health	State	Environmental State	Air quality (atmospheric emissions (GHG emissions, VOCs emitted), air quality index measurements), water quality (number of discharges that threaten existing water sources, contaminant removal efficacy of technology, natural water source constituent changes), soil health (microbiome health, soil disturbance, soil compaction), chemical use, natural water cycles (Changes to natural water flow volumes or quality)	Y	All emissions from operations are quantified into the TRACI impacts: acidification, carcinogenics, ecotoxicity, eutrophication, fossil fuel depletion, global warming, non-carcinogenics, ozone depletion, respiratory effects, smog.
Equitable Burdens	Equitable Burdens	Driver	Social Drivers	Stakeholder involvement, access to healthcare (distance to major healthcare facilities, healthcare quality), burdened population distributions, equitable access to education & information (number of industry sponsored information events, number government sponsored information events, number of mailed informational items, number of blogs, publications, and websites available to the public), equitably based policies	N	Included as part of the community livability indicator. Information not readily available.
GHG Emissions	Global Warming Potential	State	Environmental State	Methane emissions, carbon emission, NOx emissions	N	Included as part of the atmospheric emissions indicator.
Natural Water Cycles	Natural Water Cycles	Impact	Ecosystem Services	Changes to natural water flow volumes or quality	N	Irrelevant to this comparison, as each technology produces the same water products, thus having the water impacts applied.
Produced Water Discharge	Produced Water Discharge	Driver	Economic Driver	Amount of PW discharged, PW treated, Dry salts discharged	N	Irrelevant to this comparison, as each treatment technology will treat and discharge the same amount of water and salt products.
		Pressure	Environmental Pressure			

Produced Water Research	Produced Water Research	Driver	Economic Driver	Percent of Journal publications mentioning produced water	N	Irrelevant to this comparison, as research interest in PW management will not change with the technologies being used.
Property Value	Property Value	Driver	Economic Driver	Government assigned property value, sense of property value from survey results on a Likert scale	N	Information not readily available.
Public Health	Physical & Mental Well-Being	Impact	Human Well-being	Exposure to pollutants, number of hospital visits, air quality index, healthy life expectancy, access to healthcare (distance to major healthcare facilities, healthcare quality)	Y	Able to provide an impact to human health from pollutants using TRACI impacts of carcinogenics, non-carcinogenics, and respiratory effects.
	Public Health	Driver	Economic Driver			
		State	Human State			
Representation of Stakeholders	Representation of Stakeholders	Driver	Social Drivers	Number of community/academic/industry/government members active in decision making, number of stakeholder groups represented	N	Information not readily available. Irrelevant to this comparison, as community involvement will not change with the technologies being used.
Resource Management	Clean Water Access	Impact	Ecosystem Services	Number of practices in use to reduce water use, potable water source retention, non-potable water source retention, number of discharges that threaten existing water sources, increases to energy efficiency	N	Information not readily available.
	Resource Management	State	Environmental State			
Resource Use	Resource Use	Driver	Economic Driver	Water consumption, energy consumption	N	Water consumption is irrelevant to this comparison, as each technology will treat the same volume of produced water to the same levels. The impacts from energy consumption are calculated through the TRACI impacts which are metrics for the environmental health indicator.
Transportation Requirements	Transportation Requirements	Driver	Economic Driver	Distance trucks must travel for equipment supply and disposal	N	Irrelevant to this comparison, as each treatment technology will be placed in the same location with same products.
Water Quality	Waterborne Discharges	Pressure	Environmental Pressure	Number of discharges that threaten existing water sources, treatment efficacy (amount of contaminants removed), natural water source constituent changes	N	Included as part of the environmental health and access to clean water indicators. Information not readily available.

Table S69: Score of metrics and key indicators

Metric Scores

Metric	Cons. MVC+C	Avg. MVC+C	Opt. MVC+C	Cons. EDC	Avg. EDC	Opt. EDC	Cons MD+C	Avg. MD+C	Opt. MD+C	Cons MD+C w/ WH	Avg. MD+C w/ WH	Opt. MD+C w/ WH
Acidification	10	10	10	10	10	10	0	6	8	10	10	10
Ecotoxicity	10	10	10	10	10	10	0	6	8	10	10	10
Eutrophication	10	10	10	10	10	10	0	6	8	10	10	10
Fossil Fuel Depletion	10	10	10	10	10	10	0	6	8	10	10	10
Global Warming Potential	10	10	10	10	10	10	0	6	8	10	10	10
Ozone Depletion	10	10	10	0	7	9	9	10	10	10	10	10
Smog	10	10	10	10	10	10	0	6	8	10	10	10
Carcinogenics	10	10	10	10	10	10	0	6	8	10	10	10
Non-carcinogenics	10	10	10	10	10	10	0	6	8	10	10	10
Respiratory Effects	10	10	10	10	10	10	0	6	8	10	10	10
Capital Costs	10	10	10	0	9	10	8	10	10	6	9	10
Operating Costs	10	10	10	8	10	10	0	7	9	10	10	10

Key Indicator Scores

Key Indicator	Cons. MVC+C	Avg. MVC+C	Opt. MVC+C	Cons. EDC	Avg. EDC	Opt. EDC	Cons MD+C	Avg. MD+C	Opt. MD+C	Cons MD+C w/ WH	Avg. MD+C w/ WH	Opt. MD+C w/ WH
Economic Prosperity	10.0	10.0	10.0	4.0	9.5	10.0	4.0	8.5	9.5	8.0	9.5	10.0
Environmental Health	10.0	10.0	10.0	9.0	9.7	9.9	0.9	6.4	8.2	10.0	10.0	10.0
Public Health	10.0	10.0	10.0	10.0	10.0	10.0	0.0	6.0	8.0	10.0	10.0	10.0

Table S70: Technology Preference Scores for each Preference Scenario

Metric Scores

Preference Scenario	Cons. MVC+C	Avg. MVC+C	Opt. MVC+C	Cons. EDC	Avg. EDC	Opt. EDC	Cons MD+C	Avg. MD+C	Opt. MD+C	Cons MD+C w/ WH	Avg. MD+C w/ WH	Opt. MD+C w/ WH
Economics Only	10.00	10.00	10.00	4.00	9.50	10.00	4.00	8.50	9.50	8.00	9.50	10.00
Environment Only	10.00	10.00	10.00	9.00	9.70	9.90	0.90	6.40	8.20	10.00	10.00	10.00
Social Only	10.00	10.00	10.00	10.00	10.00	10.00	0.00	6.00	8.00	10.00	10.00	10.00
Even Weight	10.00	10.00	10.00	7.67	9.73	9.97	1.63	6.97	8.57	9.33	9.83	10.00
Economically Important	10.00	10.00	10.00	6.20	9.64	9.98	2.58	7.58	8.94	8.80	9.70	10.00
Socially Negligible	10.00	10.00	10.00	6.50	9.60	9.95	2.45	7.45	8.85	9.00	9.75	10.00
Environmentally Important	10.00	10.00	10.00	8.20	9.72	9.94	1.34	6.74	8.42	9.60	9.90	10.00
Economically Negligible	10.00	10.00	10.00	9.50	9.85	9.95	0.45	6.20	8.10	10.00	10.00	10.00
Socially Important	10.00	10.00	10.00	8.60	9.84	9.98	0.98	6.58	8.34	9.60	9.90	10.00
Environmentally Negligible	10.00	10.00	10.00	7.00	9.75	10.00	2.00	7.25	8.75	9.00	9.75	10.00